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A VARIATIONAL CALCULATION OF THE ELASTIC SCATTERING OF ELECTRONS BY HYDROGEN ATOMS

by

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Table of Contents

		page
I.	Introduction	1
II.	Mathematical Preliminaries	8
III.	Reduction of a Basic Fifteen-Dimensional Integral	15
IV.	Scattering from the Hartree Static Field	25
V.	The Complete Scattering	32
	A. Contribution of the Higher Discrete States	33
	B. Contribution of the Continuum States	39
VI.	Discussion of Results and Conclusions	44

Appendices:

A-I.	Evaluation of the Integral (25)	47
A-II.	Evaluation of the Static Field $W_\infty(\vec{r}_1)$	49
A-III.	Evaluation of the Integral (40)	51
A-IV.	Evaluation of the Integral (42)	53
A-V.	Evaluation of the Integral (50) for n = 2	57

Abstract

The Schwinger variational method for three-body collisions is applied to the calculation of elastic cross-sections for electron scattering from hydrogen atoms in the energy range 0 - 10 volts. Total cross-sections are obtained from the relation Q equals $\frac{4\pi}{k}$ times the imaginary part of the direct elastic scattered amplitude in the forward direction. With a Born trial field the effect on the scattering of the virtual transitions to higher states, including the continuum, can be taken into account accurately. The procedure is also applied to the calculation of the scattering from the static field of the hydrogen atom.

I. Introduction

One of the important problems of upper atmospheric and astrophysical research is the determination of the frequencies of collisions between electrons and atomic systems. Information on this subject can be obtained from a knowledge of the total cross-section, Q, and to some extent from the differential cross-section, $\sigma(\theta)$, of the collision.

The temperatures at which these collisions occur are of such a magnitude that the electron energies are of the order of a fraction of an electron volt, and at these low energies the problems associated with experimental determinations of the cross-sections become complex. Consequently there is a deficiency of experimental data. It is therefore essential to have theoretical methods for calculating the cross-sections.

A collision between an electron and an atom constitutes a many-body problem, and an exact theoretical calculation of Q and $\sigma(\theta)$ is virtually impossible. Whereas a two-body collision is characterized simply by the deflection of the incident particle by a force center, the many-body collision has associated with it several complicating features. Collisions of the latter type usually involve some reaction of the scattered particle on the atom, notably exchange and excitation phenomena, neither of which is present in purely two-body collisions. Excitation phenomena include inelastic

collisions[1,2] in which some of the energy of the incident particle is absorbed by the atomic system. It may also include purely elastic collisions in which the virtual transitions[3] of the atom to its excited states during the collision must be considered.

Exchange effects can occur when the interaction between the incident particle and one of the atomic particles is such as to cause the incident particle to be captured and the atomic particle to be ejected. If the incident and ejected particles happen to be identical, interference effects between the direct and exchange scattered waves need be considered. In this case the wave function of the system must satisfy special symmetry requirements in accordance with the Pauli principle.[4,5]

In this paper we shall consider the simplest of many-body collisions--scattering of electrons by hydrogen atoms. A successful theoretical approach to this problem can be of aid in the understanding and treatment of collisions with more complicated atomic systems.

Even here, exact calculation of the cross-sections is impossible and one must in the end resort to approximation procedures. The elastic scattering of particles by atoms can,

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1. N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1949), Second Edition, Chapter 8, sections 2, 3; Chapter 10, section 7; Chapter 11.
2. Massey and Mohr, Proc. Roy. Soc. A146, 880 (1934).
3. Ref. 1, Chapter 8, section 8.
4. Ref. 1, Chapter 8, section 4; Chapter 10, sections 5, 6.
5. Morse and Allis, Phys. Rev. 44, 269 (1933).

in certain approximations, be treated as a two-body problem. Such is the case, for example, when a Hartree field or a Fermi-Thomas statistical potential is used to represent the static field of the atom[6]. Macdougall[7] and Chandrasekhar and Breen[8] have treated the low energy collisions of electrons with hydrogen atoms in this manner, using the partial wave method of Faxén and Holtsmark[9] to determine the cross-sections. Neither exchange nor atomic excitation is taken into account in references 7 and 8.

The need for approximation procedures which are accurate and do not involve cumbersome calculations has led, in recent years, to investigations of the applicability of variational techniques to scattering problems. In collision problems, one is concerned with establishing variational methods for calculating either the phase shifts or the scattered amplitude. A knowledge of either of these quantities serves to determine the cross-sections.

Schwinger[10,11,12,13] has devised powerful variational techniques for collision problems in which stationary expressions are given for the phase shifts and for the

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6. Ref. 1, Chapter 9; Chapter 10, section 4.
7. Proc. Roy. Soc. A136, 549 (1932).
8. Astrophys. J. 103, 41 (1946).
9. Ref. 1, Chapter 2.
10. J. Schwinger, hectographed notes on nuclear physics, Harvard University, unpublished.
11. N. Marcuvitz, section IIID Recent Developments in the Theory of Wave Propagation, New York University, Institute for Mathematics and Mechanics (1949).
12. J. Schwinger and B. A. Lippman, Phys. Rev. 79, 469 (1950).
13. J. M. Blatt and J. D. Jackson, Phys. Rev. 76, 18 (1949) section II.

scattered amplitude. The method has been extended to cover three-body collisions[14]. His procedure is based on the conversion of the Schrödinger differential equation into an integral equation involving a Green's function appropriate to the boundary conditions of the scattering problem. A particular feature of Schwinger's scheme is its systematic method, based on the integral equation, for improvement of the trial wave functions to be used in the stationary expression.

Hulthèn[15], using the differential operator approach, has established a variational method in which the phase shifts may be calculated approximately. Unlike the Schwinger scheme, his method does not propose an explicit stationary expression for the phase shifts, nor does it aid in choosing trial wave functions. The calculations involved in the Schwinger method are, however, generally more complex as a result of the presence of the Green's function. Kohn[16] has developed further variational procedures for the phase shifts and scattered amplitude in many-body collision problems using methods related to Hulthèn's approach. Kato[17] has devised a variational procedure in which upper and lower bounds on the phase shifts can be calculated. He has applied the method to the determination of low energy cross-sections for electron scattering from the static (Hartree) field of the hydrogen atom.

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14. S. Borowitz and B. Friedman, Phys. Rev. 89, 441(1953).
15. L. Hulthèn, Kungl. Fysio, Sällskapets Lund Förhand 14, 21 (1944).
16. W. Kohn, Phys. Rev. 74, 1763 (1948).
17. T. Kato, Prog. Theor. Phys. 6, 394 (1951).

Calculations of electron-hydrogen cross-sections have been made by various authors using the Hulthèn and Kohn variational methods. Massey and Moiseiwitsch[18] have applied these principles to the elastic scattering of electrons by hydrogen atoms. Huang[19] has formulated his own variational method and applied it to the elastic scattering of electrons by hydrogen atoms, in which the polarization effect is considered and exchange is excluded. Massey and Moiseiwitsch[20] indicate how Huang's method may be modified to include exchange. Moiseiwitsch[21] has extended Hulthèn's procedure to inelastic collision problems and has calculated the phase shifts for the 1S - 2S excitation of the hydrogen atom by electrons.

It is the purpose of this paper to apply the Schwinger variational expression for the direct scattered amplitude to the calculation of total elastic scattering cross-sections for electron-hydrogen collisions in the energy range 0 - 10 volts.

The mathematical foundation of the variational principle as applied to electron-hydrogen collisions is briefly reviewed in section II, where the difficulty of evaluating the integrals inherent in the Schwinger scheme is noted. These integrals can be made tractable if Born trial fields are used.

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18. H. S. W. Massey and B. Moiseiwitsch, Proc. Roy. Soc. A205, 483 (1951).
19. S. S. Huang, Phys. Rev. 76, 477 (1949).
20. H. S. W. Massey and B. Moiseiwitsch, Phys. Rev. 78, 180 (1950).
21. B. Moiseiwitsch, Phys. Rev. 82, 753 (1951).

The calculations of this paper are based on Born trial fields and on a theorem relating the total elastic cross-section to the direct elastic scattered amplitude in the forward direction (section II). Cross-sections given by this theorem measure the total number of directly scattered and exchange scattered particles at infinity. The contribution of the interference between the direct and exchange scattered waves to the true elastic cross-section including exchange is estimated in section II.

Section III is devoted to reduction and simplification of the basic fifteen-dimensional integral (equation 19) of the Schwinger variational method in the Born approximation.

The accuracy of results obtained by using Born trial fields in the variational expression at these low energies is tested by first considering the scattering from the static (Hartree) field of the hydrogen atom in its ground state (section IV). In this section the cross-sections obtained with the variational method are compared with the exact cross-sections obtained by Chandrasekhar and Breen[8] and with the ordinary Born approximation cross-sections. The vast improvement that the variational method affords over the ordinary Born approximation for the static field scattering leads next to a consideration of the variational method with Born trial fields in the calculation of the scattering with complete Green's function (section V). Here the effect on the scattering

of the virtual transitions of the atom to higher discrete states and to the continuum is explicitly and accurately taken into account.

An evaluation of the results of section V is given in section VI where the contributions from the excited states and the continuum are discussed and interpreted. Some remarks are made concerning the possibility of use of bound state H^- trial wave functions.

One of the objectives of this investigation is to determine the feasibility of carrying out certain fifteen-dimensional integrals characteristic of the Schwinger variational method applied to this problem.

II. Mathematical Preliminaries

The scattering cross-section for the collision of an electron with a hydrogen atom, in which the proton is assumed to have infinite mass, can be found from the solution of the Schrödinger equation for this problem:

$$(1)\quad \left\{\nabla_1^2 + \nabla_2^2 + \frac{2mE}{\hbar^2} + \frac{2}{a_o}\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right)\right\}\Psi_o(\vec{r}_1,\vec{r}_2) = 0$$

where Ψ_o is subject to the boundary conditions:

$$(2)\quad \Psi_o(r_1 \to \infty) = e^{ik_o\vec{n}_o\cdot\vec{r}_1}\,\phi_o(\vec{r}_2) + \left(\sum_n + \int\right) f_n(\theta,\phi)\frac{e^{ik_n r_1}}{r_1}\,\phi_n(\vec{r}_2)$$

$$\Psi_o(r_2 \to \infty) = \left(\sum_n + \int\right) g_n(\theta,\phi)\frac{e^{ik_n r_2}}{r_2}\,\phi_n(\vec{r}_1) \quad .$$

The symbols in (1) and (2) have the following meaning:

$a_o = \frac{\hbar^2}{me^2}$ = radius of first Bohr orbit in hydrogen

m = mass of electron

e = charge of electron

$\hbar = \frac{h}{2\pi}$, h = Planck's constant.

$\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the incident and bound electrons, respectively, relative to the proton, and $r_{12} = |\vec{r}_1 - \vec{r}_2|$. E is the sum of the energy E_o of the bound electron in its ground state and the energy of the incident electron, $\frac{\hbar^2 k_o^2}{2m}$, where k_o is the wave number of the incident

electron. $\vec{n}_o$ is a unit vector in the direction of motion of the incident electron. $\phi_n(\vec{r}_2)$ are the wave functions, corresponding to energies E_n, of the unperturbed bound electron and k_n are wave numbers determined from conservation of energy: $E = E_n + \frac{\hbar^2 k_n^2}{2m}$. The symbol $\left(\sum_n + \int\right)$ denotes summation over discrete states and integration over continuum states. The quantities f_n and g_n defined in (2) are the direct and exchange scattering amplitudes, respectively, in the cases where k_n are real numbers.

The correct solution to the problem involves the symmetrization of Ψ_o in accordance with the Pauli principle for identical particles. A solution of (1) which satisfies this principle and the boundary conditions is $\Psi_o(\vec{r}_1,\vec{r}_2) \pm \Psi_o(\vec{r}_2,\vec{r}_1)$ where the plus and minus signs are taken for the antisymmetric and symmetric spin states, respectively. The differential cross-section is then given by

$$(3) \qquad \sigma_n = \frac{k_n}{k_o}\left[\frac{3}{4}\,|f_n - g_n|^2 + \frac{1}{4}\,|f_n + g_n|^2\right] \quad .$$

We shall not consider the evaluation of the quantities $g_n(\theta)$ in this paper. We shall be concerned, instead, with the direct scattered amplitudes f_n, and in particular with the elastic amplitude f_o for incident electron energies less than the excitation energy of the first excited state of the atomic electron. It is indicated later in this section how the

elastic cross-section, including exchange, may be estimated in terms of the direct elastic amplitude, f_o.

The procedure [14] in formulating a Schwinger variational principle involves the conversion of the differential equation (1) into an integral equation. The integral equation is made to satisfy the boundary conditions of the problem by appropriate choice of the Green's function. It can then be shown[11,14] that the following expression for f_n is stationary with respect to arbitrary variations of Ψ_o and Ψ_n about their correct values:

$$-4\pi f_n(\theta) = \frac{E \cdot H}{P - R} \tag{4}$$

where

$$E = \int e^{ik_o \vec{n}_o \cdot \vec{r}_1} \phi_o(\vec{r}_2) V(\vec{r}_1, \vec{r}_2) \overset{*}{\Psi}_n(\vec{r}_1, \vec{r}_2) d\tau_1 d\tau_2$$

$$H = \int e^{-ik_n \vec{n} \cdot \vec{r}_1} \overset{*}{\phi}_n(\vec{r}_2) V(\vec{r}_1, \vec{r}_2) \Psi_o(\vec{r}_1, \vec{r}_2) d\tau_1 d\tau_2$$

$$P = \int \Psi_o(\vec{r}_1, \vec{r}_2) V(\vec{r}_1, \vec{r}_2) \overset{*}{\Psi}_n(\vec{r}_1, \vec{r}_2) d\tau_1 d\tau_2$$

$$R = \iint \overset{*}{\Psi}_n(\vec{r}_1, \vec{r}_2) V(\vec{r}_1, \vec{r}_2) G(\vec{r}_1, \vec{r}_2, \vec{r}_1', \vec{r}_2') V(\vec{r}_1', \vec{r}_2') \Psi_o(\vec{r}_1', \vec{r}_2') d\tau_1 d\tau_2 d\tau_1' d\tau_2'$$

where G is the Green's function of the operator $\left(\nabla_1^2 + \nabla_2^2 + \frac{2mE}{\hbar^2} + \frac{2}{a_o} \cdot \frac{1}{r_2}\right)$ appropriate to the boundary conditions of the problem and is given by[14]

$$(5)\quad G(\vec{r}_1,\vec{r}_2,\vec{r}_1',\vec{r}_2') = -\left(\sum_m + \int\right) \phi_m(\vec{r}_2)\overset{*}{\phi}_m(\vec{r}_2')\frac{e^{ik_m|\vec{r}_1 - \vec{r}_1'|}}{4\pi|\vec{r}_1 - \vec{r}_1'|}$$

$$(6)\quad V(\vec{r}_1,\vec{r}_2) = \frac{2}{a_o}\left(\frac{1}{r_{12}} - \frac{1}{r_1}\right)$$

θ is the scattering angle, such that

$$(7)\qquad \cos\theta = \vec{n}_o \cdot \vec{n}$$

$\vec{n}$ being a unit vector in the scattered direction, and $\Psi_n(\vec{r}_1,\vec{r}_2)$ is the solution of (1) in the case where the electron is incident in the direction $\vec{n}$ with wave number k_n and the bound electron is in the state $\phi_n(\vec{r}_2)$.

Variational expressions for $g_n(\theta)$ are developed in reference 14.

The evaluation of the expression (4) is exceedingly difficult for all but Born trial fields. If the Born trial fields

$$(8)\qquad \Psi_o \sim e^{ik_o\vec{n}_o\cdot\vec{r}_1}\,\phi_o(\vec{r}_2)$$

$$\Psi_n \sim e^{ik_n\vec{n}\cdot\vec{r}_1}\,\phi_n(\vec{r}_2)$$

are used in (4) as first approximations, then the expression for the direct elastic scattering amplitude becomes

(9) $f_o(\theta) =$

$$\frac{-\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(\vec{r})\, d\tau}{1-\frac{\iint e^{-ik_o\vec{n}\cdot r_1}\left(\sum_m+\int\right)W_{om}(\vec{r}_1)\frac{e^{ik_m|\vec{r}_1-\vec{r}_2|}}{-4\pi|\vec{r}_1-\vec{r}_2|}W_{mo}(\vec{r}_2)e^{ik_o\vec{n}_o\cdot\vec{r}_2}\, d\tau_1 d\tau_2}{\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(\vec{r})\, d\tau}}$$

where

(10) $$W_{nm}(\vec{r}_1) \equiv \int \phi_n^*(\vec{r}_2)V(\vec{r}_1,\vec{r}_2)\phi_m(\vec{r}_2)d\tau_2$$

$$V(\vec{r}_1,\vec{r}_2) = \frac{2}{a_o}\left(\frac{1}{r_{12}} - \frac{1}{r_1}\right)$$

ϕ_m = hydrogen wave functions .

Even in this approximation, the work involved in evaluating (9) for arbitrary scattering angle θ is prohibitive. We shall therefore make use of the following formula[22] for the total elastic cross-section:

(11) $$Q = \frac{4\pi}{k_o}\,\mathrm{Im}\, f_o(0)$$

where Im $f_o(0)$ is the imaginary part of the elastic scattering amplitude in the forward direction $\vec{n} = \vec{n}_o$.

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22. The existence of this formula was brought to our attention by Dr. E. Gerjuoy. A proof of (11) for problems in which exchange is not possible has been given by E. Feenberg, Phys. Rev. 40, 40 (1932). Dr. Gerjuoy has submitted a proof to us (private communication) in which (11) is shown to hold for problems where exchange is possible.

If we designate the incident electron by # 1 and the bound electron by # 2, then Q in (11) measures the number of # 1 particles plus the number of # 2 particles appearing in the elastic scattered wave at infinity per unit time per unit incident flux. Thus

$$Q = \int \left(|f_o|^2 + |g_o|^2 \right) d\Omega \tag{12}$$

where the integration in (12) is carried out over all solid angle Ω .

On the other hand the true total elastic cross-section in which exchange is included is given by (see 3)

$$Q' = \int \sigma_o d\Omega = \int \left(\tfrac{3}{4}|f_o - g_o|^2 + \tfrac{1}{4}|f_o + g_o|^2 \right) d\Omega \tag{13}$$

which may be written as

$$Q' = Q - \tfrac{1}{2} \int (g_o \overset{*}{f}_o + f_o \overset{*}{g}_o) d\Omega \quad . \tag{14}$$

The maximum value of the second term on the right side of (14) can be obtained as follows: Let

$$f_o = ae^{i\alpha} \quad , \quad g_o = be^{i\beta} \quad . \tag{15}$$

Then

$$J \equiv \tfrac{1}{2} \int (g_o \overset{*}{f}_o + f_o \overset{*}{g}_o) d\Omega = \int ab \cos(\alpha - \beta) d\Omega \quad . \tag{16}$$

Thus $|J| \leq \int ab d\Omega$. From (12) and (15) $Q = \int (a^2 + b^2) d\Omega$. If we let $a^2 + b^2 = \lambda$, then $Q = \int \lambda \, d\Omega$ and

$$(17) \qquad |J| \leq \int a\sqrt{\lambda - a^2}\, d\Omega \quad .$$

The maximum value of the right side of (17) occurs when $a = \sqrt{\frac{\lambda}{2}}$. Hence the maximum value of the right side of (17) is $\int \frac{\lambda}{2}\, d\Omega = \frac{1}{2}Q$, so that $|J| \leq \frac{1}{2}Q$. Then (14) shows that the total elastic cross-section, including exchange, lies somewhere between $\frac{3Q}{2}$ and $\frac{Q}{2}$, depending on the phase relation between f_o and g_o.

The cross-sections, Q, which we shall calculate in this paper are therefore in error by at most $\pm \frac{Q}{2}$ with respect to the true exchange elastic cross-section. In view of the paucity of experimental data on the cross-sections in the range 0 - 10 volts, we do not regard this error as serious in the interpretation of the results of the calculations.

III. Reduction of a Basic Fifteen Dimensional Integral

Before considering the application of (9) to the static field scattering, it will be advantageous to simplify the following quantity which appears in the denominator of (9):

$$I(\theta) \equiv \iint e^{-ik_o\vec{n}\cdot\vec{r}_1}\left(\sum_m + \int\right) W_{om}(\vec{r}_1)\frac{e^{ik_m|\vec{r}_1-\vec{r}_2|}}{4\pi|\vec{r}_1-\vec{r}_2|} W_{mo}(\vec{r}_2)e^{ik_o\vec{n}_o\cdot\vec{r}_2}\, d\tau_1 d\tau_2$$

This simplification will then allow us to proceed directly to a consideration of the static field scattering (section IV) and the complete scattering (section V), both with Born trial fields.

For this purpose we shall use the Fourier integral representation of the Green's function[23]

$$\frac{e^{ik_m|\vec{r}_1-\vec{r}_2|}}{4\pi|\vec{r}_1-\vec{r}_2|} = \frac{1}{8\pi^3}\int \frac{e^{i\vec{k}'\cdot(\vec{r}_1-\vec{r}_2)}}{k'^2 - k_m^2}\, d\tau_{k'} \quad . \tag{18}$$

Here $\vec{k}'$ is any propagation vector of magnitude k' and $d\tau_{k'}$ is the volume element in $\vec{k}'$ space.

In order to obtain only outgoing waves ($\frac{e^{ik_m r_1}}{r_1}$ rather than $\frac{e^{-ik_m r_1}}{r_1}$ for r_1 large) and thereby satisfy the boundary conditions of the problem, the singularities $k' = \pm k_m$ in the integrand of (18) must be circumvented in the manner indicated in figure 1.[23]

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23. L. I. Schiff, "Quantum Mechanics" (McGraw Hill Co. 1949), First Edition, pp. 161,62.

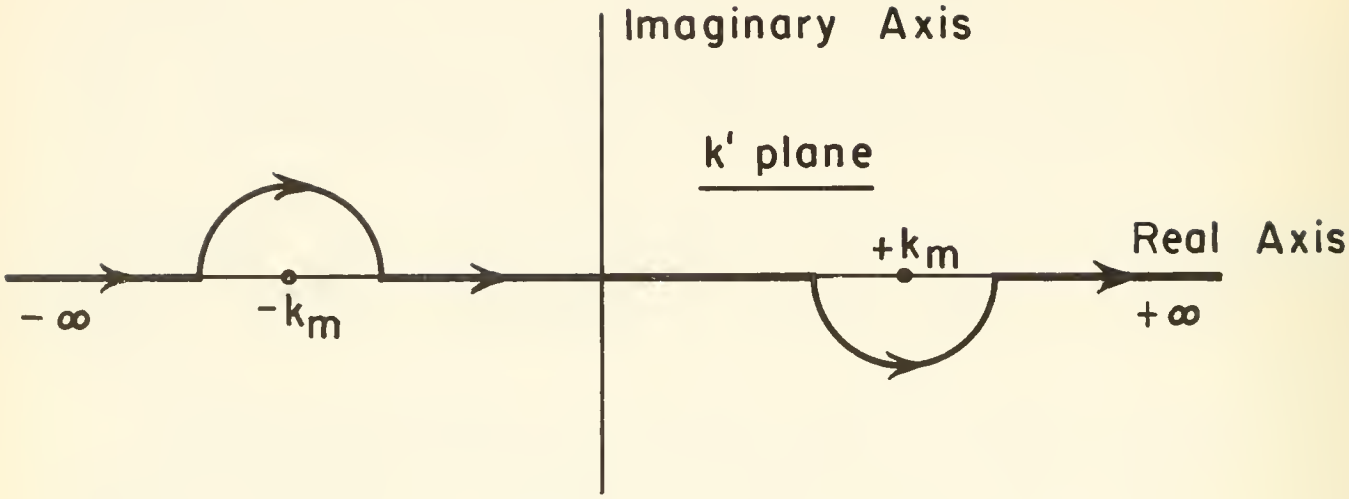

Fig. 1

This statement is the basis for the procedure used in carrying out certain integrations appearing in subsequent sections.

We state without proof that the Fourier representation (18) is valid when k_m is pure imaginary. The singularities are then located on the imaginary axis and an elementary contour integration in (18) will show that both left and right hand members agree. This fact is of importance when the virtual transitions of the atom to higher states are considered (section V).

Substitution of (18) and (10) into the expression for I yields

$$(19) \quad I(\theta) = \frac{1}{2\pi^3 a_o^2} \int e^{i(\vec{k}'-k_o\vec{n}).\vec{r}_1} e^{i(k_o\vec{n}_o-\vec{k}')\cdot\vec{r}_2} \left(\frac{1}{r_{13}} - \frac{1}{r_1}\right)\left(\frac{1}{r_{24}} - \frac{1}{r_2}\right) \Phi \, dt$$

where

$$\Phi = \left(\sum_m + \int\right) \frac{\overset{*}{\phi}_o(\vec{r}_3)\phi_m(\vec{r}_3)\phi_o(\vec{r}_4)\overset{*}{\phi}_m(\vec{r}_4)}{k'^2 - k_m^2}$$

and

$$dt = d\tau_1\, d\tau_2\, d\tau_3\, d\tau_4\, d\tau_{k'} \quad .$$

The geometry in figure 2 will aid in the simplification of this fifteen dimensional integral.

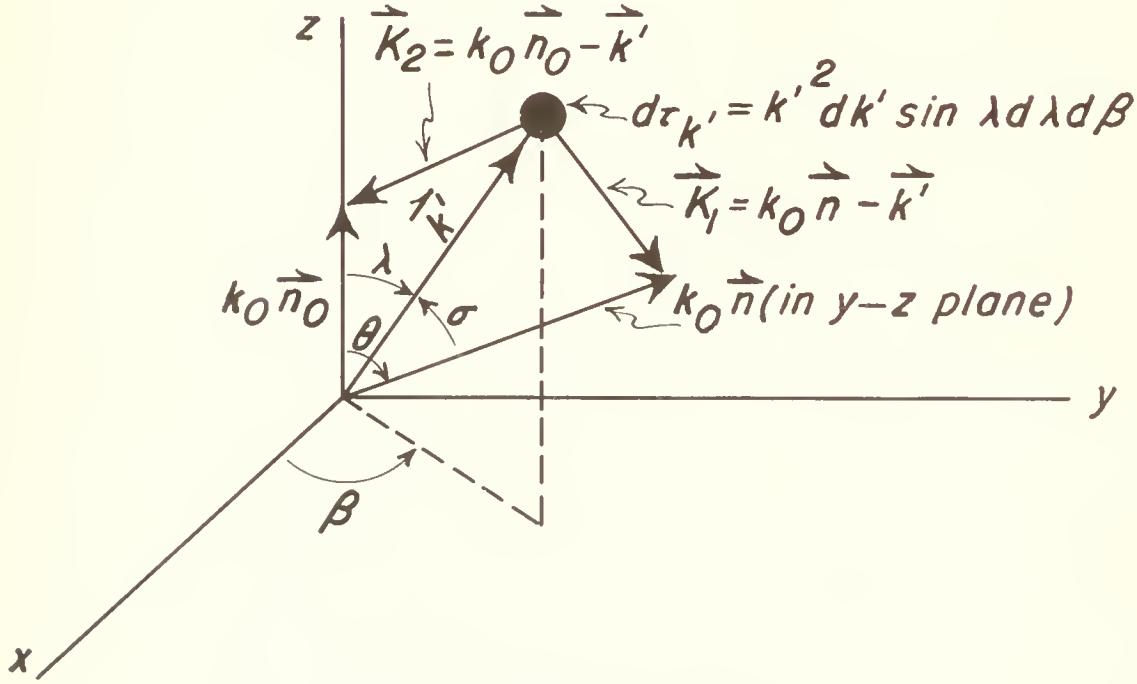

Fig. 2

From figure 2, we have

$$K_1^2 = |k_o\vec{n} - \vec{k'}|^2 = k'^2 + k_o^2 - 2k_o k' \cos\sigma$$

(20)

$$K_2^2 = |k_o\vec{n}_o - \vec{k'}|^2 = k'^2 + k_o^2 - 2k_o k' \cos\lambda \quad .$$

A relation between σ and θ, λ. β can be established as follows:

$$k_o\vec{n} = (0,\ k_o \sin\theta,\ k_o \cos\theta)$$

$$\vec{k'} = (k' \sin\lambda \cos\beta,\ k' \sin\lambda \sin\beta,\ k' \cos\lambda) \quad .$$

Hence

$$\vec{k'}\cdot k_o\vec{n} = k'k_o \cos\sigma = k'k_o \sin\lambda \sin\beta \sin\theta$$

$$+ k'k_o \cos\lambda \cos\theta$$

so that

(21) $$\cos\sigma = \cos\lambda \cos\theta + \sin\lambda \sin\beta \sin\theta \quad .$$

Equation (19) now becomes, with $\alpha = \frac{2}{a_o}$,

(22) $$I = \frac{\alpha^2}{8\pi^3}\left\{I_1 - I_2 - I_3 + I_4\right\}$$

where

(22-1) $$I_1 = \int \frac{e^{-i\vec{K}_1\cdot\vec{r}_1}}{r_{13}} \frac{e^{i\vec{K}_2\cdot\vec{r}_2}}{r_{24}} \Phi\, dt$$

(22-2) $$I_2 = \int \frac{e^{-i\vec{K}_1\cdot\vec{r}_1}}{r_1} \frac{e^{i\vec{K}_2\cdot\vec{r}_2}}{r_{24}} \Phi\, dt$$

(22-3) $$I_3 = \int \frac{e^{-i\vec{K}_1\cdot\vec{r}_1}}{r_{13}} \frac{e^{i\vec{K}_2\cdot\vec{r}_2}}{r_2} \Phi\, dt$$

$$(22\text{-}4) \qquad I_4 = \int \frac{e^{-i\vec{K}_1\cdot\vec{r}_1}}{r_1} \frac{e^{i\vec{K}_2\cdot\vec{r}_2}}{r_2} \Phi\, dt \quad .$$

We shall make use of the following formulae[24]:

$$(23) \qquad \int \frac{e^{i\vec{K}\cdot\vec{r}_1}}{r_{12}} d\tau_1 = \frac{4\pi}{K^2} e^{i\vec{K}\cdot\vec{r}_2} \quad , \quad \int \frac{e^{i\vec{K}\cdot\vec{r}_1}}{r_1} d\tau_1 = \frac{4\pi}{K^2} \quad .$$

We shall also use the orthonormality relation for the hydrogen wave functions:

$$(24) \qquad \int \phi_o(\vec{r})\, \overset{*}{\phi}_m(\vec{r})\, d\tau = \delta_{om} = \begin{matrix} 1 \text{ for } m = 0 \\ 0 \text{ for } m \neq 0 \end{matrix} \quad .$$

Finally we shall use the result[25]

$$(25) \qquad \int e^{i\vec{K}\cdot\vec{r}} \,|\phi_o(\vec{r})|^2 d\tau = \frac{a^4}{(a^2+K^2)^2} \quad , \quad a = \frac{2}{a_o} \quad .$$

With (23), (24) and (25), equations (22-1) through (22-4) simplify considerably. The result is easily seen to be

$$(26\text{-}1) \quad I_1 = 16\pi^2 a^8 \int \frac{d\tau_{k'}}{(k'^2-k_o^2)K_1^2K_2^2(a^2+K_1^2)^2(a^2+K_2^2)^2}$$

$$+ 16\pi^2\left(\sum_{m>0} + \int\right)\int \frac{d\tau_{k'}}{(k'^2-k_m^2)K_1^2K_2^2} \int e^{-i\vec{K}_1\cdot\vec{r}_3}\, \overset{*}{\phi}_o(\vec{r}_3)\phi_m(\vec{r}_3)\, d\tau_3$$

$$\cdot \int e^{i\vec{K}_2\cdot\vec{r}_4}\, \phi_o(\vec{r}_4)\overset{*}{\phi}_m(\vec{r}_4)\, d\tau_4$$

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24. H. A. Bethe, Ann. der Phys., 5, 325 (1930)
L. I. Schiff, loc.cit. p. 201.

25. See appendix AI.

$$(26\text{-}2) \qquad I_2 = 16\pi^2 a^4 \int \frac{d\tau_{k'}}{(k'^2-k_o^2)K_1^2K_2^2(a^2 + K_2^2)^2}$$

$$(26\text{-}3) \qquad I_3 = 16\pi^2 a^4 \int \frac{d\tau_{k'}}{(k'^2-k_o^2)K_1^2K_2^2(a^2 + K_1^2)^2}$$

$$(26\text{-}4) \qquad I_4 = 16\pi^2 \int \frac{d\tau_{k'}}{(k'^2-k_o^2)K_1^2K_2^2} \quad .$$

Substitution of (26-1) through (26-4) into (22) gives following result after collecting and simplifying terms:

$$(27) \qquad I(\theta) = \frac{2a^2}{\pi} \int \frac{d\tau_{k'}}{(k'^2-k_o^2)} \cdot \frac{(2a^2 + K_1^2)}{(a^2 + K_1^2)^2} \cdot \frac{(2a^2 + K_2^2)}{(a^2 + K_2^2)^2}$$

$$+ \frac{2a^2}{\pi}\left(\sum_{n>0} + \int\right)\int \frac{d\tau_{k'}}{(k'^2-k_n^2)K_1^2K_2^2} \int e^{-i\vec{K}_1\cdot\vec{r}_3}\, \overset{*}{\phi}_o(\vec{r}_3)\phi_n(\vec{r}_3)d\tau_3$$

$$\cdot \int e^{i\vec{K}_2\cdot\vec{r}_4}\, \phi_o(\vec{r}_4)\overset{*}{\phi}_n(\vec{r}_4)d\tau_4 \quad .$$

The evaluation of (27) for arbitrary scattering angle θ is formidable. We shall, from this point on, consider only $\theta = 0$ with a view ultimately to applying the cross-section theorem (11).

For $\theta = 0$, equations (20) and (21) give

$$(28) \qquad \begin{aligned} \cos\sigma &= \cos\lambda \\ K_1^2 = K_2^2 &\equiv K^2 = k'^2 + k_o^2 - 2k_o k' \cos\lambda \end{aligned}$$

and from figure 2

(29) $$\vec{K}_1 = \vec{K}_2 \equiv \vec{K} = k_o\vec{n}_o - \vec{k}'$$

(27) then becomes

(30) $$I(0) = \frac{2a^2}{\pi}\int \frac{d\tau_{k'}}{(k'^2-k_o^2)} \frac{(2a^2+K^2)^2}{(a^2+K^2)^4}$$

$$+ \frac{2a^2}{\pi}\left(\sum_{n>0} + \int\right)\int \frac{d\tau_{k'}}{(k'^2-k_n^2)K^4}\left|\int e^{i\vec{K}\cdot\vec{r}}\,\phi_o(\vec{r})\,\overset{*}{\phi}_n(\vec{r})\,d\tau\right|^2$$

where $\sum_n + \int$ in (30) really stands for $\sum_{n\ell m} + \int_0^\infty dk \sum_{\ell m}$ and ϕ_n is either $\phi_{n\ell m}$ (discrete state wave function) or $\phi_{k\ell m}$ (continuum state wave function). The meanings of n, ℓ, m, and k are: n, principal quantum number; ℓ, angular momentum quantum number; m, magnetic quantum number; k, wave number of atomic electron when in continuum.

If, then, we define the matrix elements

(31) $$\varepsilon_{o,n\ell m} = \int e^{i\vec{K}\cdot\vec{r}}\,\phi_o(\vec{r})\,\overset{*}{\phi}_{n\ell m}(\vec{r})\,d\tau$$

$$\varepsilon_{o,k\ell m} = \int e^{i\vec{K}\cdot\vec{r}}\,\phi_o(\vec{r})\,\overset{*}{\phi}_{k\ell m}(\vec{r})\,d\tau$$

(32) $$|\varepsilon_{o,n}(K)|^2 \equiv \sum_{\ell m} |\varepsilon_{o,n\ell m}|^2$$

$$|\varepsilon_{o,k}(K)|^2 \equiv \sum_{\ell m} |\varepsilon_{o,k\ell m}|^2$$

(30) may be written as

$$(33)\quad I(0) = \frac{2a^2}{\pi}\int \frac{d\tau_{k'}}{(k'^2-k_o^2)}\,\frac{(2a^2+K^2)^2}{(a^2+K^2)^4}$$

$$+\frac{2a^2}{\pi}\sum_{n>0}\int \frac{d\tau_{k'}}{(k'^2-k_n^2)K^4}\,|\varepsilon_{o,n}(K)|^2$$

$$+\frac{2a^2}{\pi}\int_0^\infty dk\int \frac{d\tau_{k'}}{(k'^2-k_c^2)K^4}\,|\varepsilon_{o,k}(K)|^2$$

where k_n and k_c are wave numbers determined from conservation of energy:

$$(34)\quad \begin{aligned} E &= E_n + \frac{\hbar^2 k_n^2}{2m}\ ; \quad E_n = -\frac{e^2}{2a_o(n+1)^2} \qquad (n = 0,1,2,\ldots) \\ E &= E_c + \frac{\hbar^2 k_c^2}{2m}\ ; \quad E_c = \frac{\hbar^2 k^2}{2m} \end{aligned}$$

E_n and E_c being, respectively, the discrete energy levels of the hydrogen atom and the energy of the atomic electron when in the continuum with a wave number k. With $E = E_o + \frac{\hbar^2 k_o^2}{2m}$, (34) gives

$$(35)\quad \begin{aligned} k_n^2 &= k_o^2 - \frac{1}{a_o^2}\left[1 - \frac{1}{(n+1)^2}\right] \qquad n = 0,1,2,\ldots \\ k_c^2 &= k_o^2 - \frac{1}{a_o^2}\left[1 + (ka_o)^2\right] \qquad k = 0 \text{ to } \infty \text{ continuously.} \end{aligned}$$

If v is the velocity of the incident electron, then

$k_o = \frac{mv}{\hbar}$ and $k_o a_o = \sqrt{\frac{2ma_o^2}{\hbar^2}} \cdot \sqrt{\frac{1}{2}mv^2}$ so that

$$k_o a_o = \sqrt{\frac{2mea_o^2}{\hbar^2}} \cdot \sqrt{\frac{\text{volts}}{300}} = \sqrt{\frac{a_o}{150e}} \cdot \sqrt{\text{volts}} \quad .$$

With the accepted values for e and a_o, we find

$$k_o a_o = .271 \sqrt{\text{volts}} \quad . \tag{36}$$

For convenience of future reference, we collect the important results of this section:

$$I(0) = I_o + \sum_{n>0} I_n + I_c \tag{37}$$

where:

$$I_o = \frac{2a^2}{\pi} \int \frac{d\tau_{k'}}{(k'^2 - k_o^2)} \frac{(2a^2 + K^2)^2}{(a^2 + K^2)^4}$$

$$I_n = \frac{2a^2}{\pi} \int \frac{d\tau_{k'}}{(k'^2 - k_n^2) K^4} |\varepsilon_{o,n}(K)|^2$$

$$I_c = \frac{2a^2}{\pi} \int_0^\infty dk \int \frac{d\tau_{k'}}{(k'^2 - k_c^2) K^4} |\varepsilon_{o,k}(K)|^2$$

$$|\varepsilon_{o,n}(K)|^2 = \sum_{\ell m} \left| \int e^{i\vec{K}\cdot\vec{r}} \phi_o(\vec{r}) \overset{*}{\phi}_{n\ell m}(\vec{r}) \, d\tau \right|^2$$

$$|\varepsilon_{o,k}(K)|^2 = \sum_{\ell m} \left| \int e^{i\vec{K}\cdot\vec{r}} \phi_o(\vec{r}) \overset{*}{\phi}_{k\ell m}(\vec{r}) \, d\tau \right|^2$$

$$d\tau_{k'} = k'^2 dk' \sin\lambda \, d\lambda \, d\beta$$

$$K^2 = k'^2 + k_o^2 - 2k'k_o \cos\lambda$$

$$\vec{K} = k_o\vec{n}_o - \vec{k}'$$

$$k_n^2 = k_o^2 - \frac{1}{a_o^2}\left[1 - \frac{1}{(n+1)^2}\right] \quad (n = 0,1,2,\ldots)$$

$$k_c^2 = k_o^2 - \frac{1}{a_o^2}\left[1 + (ka_o)^2\right] \quad (k = 0 \text{ to } \infty \text{ continuously})$$

$$\alpha = \frac{2}{a_o}$$

$$k_o a_o = .271\sqrt{\text{incident voltage}}$$

$\phi_{n\ell m}$, $\phi_{k\ell m}$: bound state and continuum hydrogen wave functions, respectively.

IV. Scattering from the Hartree Static Field

The Hartree static field potential between an electron and a hydrogen atom in its ground state is the expectation value of the interaction potential

$$\frac{2}{a_o}\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right) : W_{oo}(\vec{r}_1) = \frac{2}{a_o}\int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)|\phi_o(\vec{r}_2)|^2 d\tau_2, \text{ (see 10).}$$

The Schwinger variational expression for the amplitude associated with electron scattering from this field is obtained from (9) with only the term m = 0 retained in the denominator:

$$(38)\quad f(\theta) = \frac{-\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(\vec{r})\, d\tau}{1-\dfrac{\iint e^{-ik_o\vec{n}\cdot\vec{r}_1}\, W_{oo}(\vec{r}_1)\dfrac{e^{ik_o|\vec{r}_1-\vec{r}_2|}}{-4\pi|\vec{r}_1-\vec{r}_2|}\, W_{oo}(\vec{r}_2)\, e^{ik_o\vec{n}_o\cdot\vec{r}_2}\, d\tau_1 d\tau_2}{\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(\vec{r})\, d\tau}}$$

where we have dropped the subscript 0 on $f(\theta)$ since static field scattering implies the existence of only elastic collisions.

(38) is the usual Schwinger expression (with Born trial fields) for a two body scattering process, in which a particle is deflected by a potential center $W_{oo}(\vec{r})$. The numerator of (38) is the first Born approximation for the amplitude for scattering from the static field $W_{oo}(\vec{r})$ [26].

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26. Mott and Massey, loc.cit. Chapter 7, equation 5.

The static potential $W_{oo}(\vec{r})$ is evaluated in appendix AII. The result is the spherically symmetric attractive potential

$$W_{oo}(r) = -\frac{2}{a_o}\left(\frac{1}{a_o} + \frac{1}{r}\right)e^{-2r/a_o} \quad . \tag{39}$$

The numerator of (38) is evaluated in appendix AIII and the result obtained is

$$-\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(r)\,d\tau = \alpha\frac{(2\alpha^2 + K^2)}{(\alpha^2 + K^2)^2} \quad , \tag{40}$$

where

$$K = |k_o\vec{n}_o - k_o\vec{n}| = 2k_o \sin\frac{\theta}{2} \; ; \quad \alpha = \frac{2}{a_o} \; ; \quad \cos\theta = \vec{n}_o\cdot\vec{n} \quad .$$

The differential cross-section for scattering from the static field, in the first Born approximation, is then given by the square of (40):

$$\sigma(\theta) = \frac{\alpha^2(2\alpha^2 + 4k_o^2 \sin^2\frac{\theta}{2})^2}{(\alpha^2 + 4k_o^2 \sin^2\frac{\theta}{2})^4} \quad . \tag{40a}$$

The total cross-section is obtained from

$$Q = 2\pi\int_0^\pi \sigma(\theta)\sin\theta\, d\theta \quad .$$

The result for the total cross-section for scattering from the static field in the first Born approximation is[27]

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27. Mott and Massey, loc.cit. Chapter 9, section 3.

$$(40b) \qquad Q = (4\pi a_o^2)\,\frac{7(k_o a_o)^4 + 18(k_o a_o)^2 + 12}{12[1+(k_o a_o)^2]^3} \quad .$$

We shall have occasion to refer to (40b) later in this section.

Define

$$(41) \quad D(\theta) = \iint e^{-ik_o\vec{n}\cdot\vec{r}_1}\, W_{oo}(\vec{r}_1)\frac{e^{ik_o|\vec{r}_1-\vec{r}_2|}}{4\pi|\vec{r}_1-\vec{r}_2|}\, W_{oo}(\vec{r}_2)e^{ik_o\vec{n}_o\cdot\vec{r}_2}\, d\tau_1 d\tau_2 \; .$$

Since $D(\theta)$ is the $m = 0$ term in the denominator of equation (9), its value for $\theta = 0$ is given by the $m = 0$ term in (37). Thus

$$(42) \qquad D(0) = I_o = \frac{2a^2}{\pi}\int \frac{d\tau_{k'}}{(k'^2 - k_o^2)} \cdot \frac{(2a^2 + K^2)^2}{(a^2 + K^2)^4} \quad ,$$

where

$$K^2 = k'^2 + k_o^2 - 2k'k_o \cos\lambda$$

$$d\tau_{k'} = k'^2 dk' \sin\lambda\, d\lambda\, d\beta \quad .$$

Indeed if we insert the Fourier resolution for $\dfrac{e^{ik_o|\vec{r}_1-\vec{r}_2|}}{4\pi|\vec{r}_1-\vec{r}_2|}$, (18), into the expression for $D(\theta)$ we obtain for $\vec{n} = \vec{n}_o$:

$$D(0) = \frac{1}{8\pi^3}\int \frac{d\tau_{k'}}{k'^2 - k_o^2}\int e^{-i\vec{K}\cdot\vec{r}_1}\, W_{oo}(\vec{r}_1)d\tau_1 \int e^{i\vec{K}\cdot\vec{r}_2}\, W_{oo}(\vec{r}_2)d\tau_2$$

where $\vec{K} \equiv k_o\vec{n}_o - \vec{k}'$. If now we apply the result in (40) to each of the last two integrals, then (42) follows directly.

(42) is evaluated in appendix AIV:

$$D(0) = I_o = 4\pi a_o[A + iB] \tag{43}$$

where

$$A = \frac{39(k_o a_o)^4 + 106(k_o a_o)^2 + 75}{96[1 + (k_o a_o)^2]^3}$$

(43a)

$$B = \frac{k_o a_o}{12} \cdot \frac{7(k_o a_o)^4 + 18(k_o a_o)^2 + 12}{[1 + (k_o a_o)^2]^3} \quad .$$

We are now in a position to apply the cross-section theorem, (11), to the static field scattering. It should be mentioned that replacing the hydrogen atom by its static field precludes the possibility of exchange, so that the exchange scattered amplitude $g_o(\theta)$ is identically zero. A comparison of equations (12) and (13) shows that in this case $Q' = Q$, so that the cross-section theorem now gives the true cross-section and the statements made in the last paragraph of section II do not apply here.

For $\theta = 0$, (40) gives

$$-\frac{1}{4\pi} \int_{\theta=0} e^{ik_o(\vec{n}_o - \vec{n}) \cdot \vec{r}} W_{oo}(r) d\tau = a_o \quad . \tag{44}$$

Then (38) becomes

$$f(0) = \frac{a_o}{1 + \frac{D(0)}{-4\pi a_o}} = \frac{a_o}{1 - (A + iB)} \quad . \tag{45}$$

Then

$$Q = \frac{4\pi}{k_o} \operatorname{Im} f(0) = \frac{4\pi}{k_o} \operatorname{Im} \frac{a_o}{(1-A)-iB} = \frac{4\pi a_o^2}{k_o a_o} \frac{B}{(1-A)^2 + B^2} \quad .$$

So

$$Q = \frac{4\pi a_o^2 B'}{(1-A)^2 + B^2} \tag{46}$$

where

$$B' = \frac{B}{k_o a_o} = \frac{7(k_o a_o)^4 + 18(k_o a_o)^2 + 12}{12[1 + (k_o a_o)^2]^3} \quad .$$

If we compare the numerator of (46) with (40b), we see that it is precisely the total cross-section for scattering from the static field in the first Born approximation. The denominator of (46) is therefore to be regarded as a correction factor to this scattering, introduced by the variational method.

The following table gives a comparison of the results of the first Born approximation cross-section (40b), the variational cross-section (46), and the exact cross-section obtained by Chandrasekhar and Breen[8] by numerical integration of the radial Schrödinger equation using the potential $W_{oo}(r)$:

Table 1 (cross-sections in units of $4\pi a_o^2$)

volts	$k_o a_o$	Q (ordinary Born-static field)	Q (variational-static field)	Q^{28} (exact-static field)
.135	.1	.99	15.66	44.50
.54	.2	.95	8.88	17.00
1.21	.3	.88	5.17	8.28
3.38	.5	.72	2.19	2.99
6.75	.707	.56	1.15	1.42
9.45	.835	.48	.83	.98

It is quite apparent that the variational method, with Born trial fields, gives far better results than the ordinary Born approximation, as far as the static field scattering is concerned.

It is interesting to observe that the quantity $\frac{D(\theta)}{4\pi}$ is precisely the 2nd Born approximation to the scattering amplitude for scattering from the static field $W_{oo}(\vec{r})$, so that the amplitude $f(\theta)$ reads, to second order,

$$(47) \qquad f(\theta) = -\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(\vec{r})\, d\tau + \frac{D(\theta)}{4\pi} \quad .$$

If now we apply the cross-section theorem (11) to (47) we find with (44) and (43),

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28. These cross-sections were obtained from the δ_o and δ_1 phase shifts tabulated in ref. 8, using the formula

$$Q = 4\pi a_o^2/(k_o a_o)^2 \left\{ \sin^2\delta_o + 3\sin^2\delta_1 \right\} \quad .$$

$$Q = \frac{4\pi}{k_o} \operatorname{Im}\left\{ a_o + a_o(A+Bi) \right\}$$

or

$$Q = \frac{4\pi a_o^2}{k_o a_o} \cdot B = 4\pi a_o^2 \cdot B' \tag{48}$$

which agrees exactly with the numerator of (46). Thus the cross-section theorem applied to the scattered amplitude in the <u>second</u> Born approximation gives back the total cross-section for scattering from the static field in the <u>first</u> Born approximation (see (40b)), whereas the theorem applied to the variational expression for the scattered amplitude, (38), gives the first Born total cross-section divided by a correction factor (see (46)). The variational method should therefore give better results than the second Born approximation, as far as use of the cross-section theorem is concerned, and indeed table 1 confirms this.

V. The Complete Scattering

The complete elastic scattering amplitude, with Born trial fields, is given by the expression (9). The contribution of the higher states (discrete and continuum) to the scattering is determined by the terms $\left(\sum_{m>0} + \int\right)$ in the double integral of the denominator of (9). This double integral, I, has been reduced and simplified for $\theta = 0$ in section III, and the result for I(0) is given in equation (37). (37) forms the starting point for the work of this section. We shall, in this section, evaluate the terms I_n $(n > 0)$ and I_c defined in (37). I_o has already been evaluated (equation (43) of section IV and appendix AIV).

The evaluation of I_n and I_c depends on a knowledge of the matrix elements $|\varepsilon_{o,n}(K)|^2$ and $|\varepsilon_{o,k}(K)|^2$ defined in (37). These matrix elements have been evaluated by Wentzel[29] and Bethe[30], and the results are[30]:

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29. Wentzel, Z.f. Phys. 58, 349 (1929).
30. H. A. Bethe, Ann. der Phys. 5, 325 (1930), see pp. 341-344.

$$|\varepsilon_{o,n}(K)|^2 = \frac{K^2}{a^2}\, 2^{10}\, (n+1)^7 \left[\frac{1}{3}\left\{(n+1)^2 - 1\right\} + \frac{4K^2}{a^2}(n+1)^2\right]$$

$$\cdot \frac{\left[n^2 + \frac{4K^2}{a^2}(n+1)^2\right]^{n-2}}{\left[(n+2)^2 + \frac{4K^2}{a^2}(n+1)^2\right]^{n+4}}$$

(49)

$$|\varepsilon_{o,k}(K)|^2 = \frac{4kK^2 a^6 \left[K^2 + \frac{1}{3}\left(\frac{a^2}{4} + k^2\right)\right]}{\left[(K+k)^2 + \frac{a^2}{4}\right]^3 \left[(K-k)^2 + \frac{a^2}{4}\right]^3}$$

$$\cdot \frac{e^{-\frac{a}{k}\tan^{-1}\frac{\alpha k}{K^2 + \frac{a^2}{4} - k^2}}}{1 - e^{-\pi a/k}}$$

$$\alpha = 2/a_o \quad .$$

A. <u>Contribution of the Higher Discrete States</u>

The contributions of the higher discrete states are governed by the quantities (see (37))

(50) $$I_n = \frac{2a^2}{\pi} \int \frac{d\tau_{k'}}{(k'^2 - k_n^2)K^4} |\varepsilon_{o,n}(K)|^2 \quad , \qquad n > 0$$

where

$$k_n^2 = k_o^2 - \frac{1}{a_o^2}\left[1 - \frac{1}{(n+1)^2}\right]$$

$$K^2 = k'^2 + k_o^2 - 2k'k_o \cos\lambda$$

$$d\tau_{k'} = k'^2 dk' \sin\lambda\, d\lambda\, d\beta \quad .$$

The methods used in evaluating the quantities I_1, I_2, I_3,... are very much the same except for differences in algebraic details. In appendix AV we outline the method in some detail for the case I_2. The results for I_1, I_2, and I_3 are the following:

$$I_1 = (4\pi a_o)\,\frac{2^{16}}{3^{10}}\left[J(\lambda_1,\tau_1)-\lambda_1^2 N_1(\lambda_1,\tau_1)-\frac{\lambda_1^4}{2}N_2(\lambda_1,\tau_1)\right.$$
$$\left.-\frac{\lambda_1^6}{3}N_3(\lambda_1,\tau_1)-\frac{\lambda_1^8}{4}N_4(\lambda_1,\tau_1)\right]$$

$$I_2 = (4\pi a_o)\,\frac{3^6}{2^{12}}\left[J(\lambda_2,\tau_2)-\lambda_2^2 N_1(\lambda_2,\tau_2)-\frac{\lambda_2^4}{2}N_2(\lambda_2,\tau_2)\right.$$
$$\left.-\frac{\lambda_2^6}{3}N_3(\lambda_2,\tau_2)-\frac{\lambda_2^8}{4}N_4(\lambda_2,\tau_2)+\lambda_2^{10}N_5(\lambda_2,\tau_2)\right] \tag{51}$$

$$I_3 = (4\pi a_o)\,\frac{9\cdot 10^{23}}{5^{13}}\left[J(\lambda_3,\tau_3)-\lambda_3^2 N_1(\lambda_3,\tau_3)-\frac{\lambda_3^4}{2}N_2(\lambda_3,\tau_3)\right.$$
$$-\frac{\lambda_3^6}{3}N_3(\lambda_3,\tau_3)-\frac{\lambda_3^8}{4}N_4(\lambda_3,\tau_3)$$
$$\left.+\frac{116}{45}\lambda_3^{10}N_5(\lambda_3,\tau_3)-\frac{32}{27}\lambda_3^{12}N_6(\lambda_3,\tau_3)\right]$$

where

$$N_i(\lambda,\tau) = \frac{1}{\pi z_o}\int_{-\infty}^{\infty} \frac{\zeta d\zeta}{(\zeta^2+\tau^2)} \frac{1}{[\lambda^2+(\zeta-z_o)^2]^i} \quad (i = 1,\ldots,6)$$

$$= -\frac{1}{(i-1)}\frac{\partial N_{i-1}}{\partial \lambda^2} \quad (i = 2,\ldots,6) \qquad \text{and}$$

(52)

$$J(\lambda,\tau) = \frac{1}{\pi z_o}\int_{-\infty}^{\infty} \frac{\zeta d\zeta}{(\zeta^2+\tau^2)} \ln \frac{\lambda^2+(\zeta-z_o)^2}{(\zeta-z_o)^2}$$

$$= \int_0^{\lambda^2} N_1(\lambda,\tau)d\lambda^2$$

with $\zeta = k'a_o$, and

$$\tau_1^2 = -(k_1a_o)^2 = \frac{3}{4} - z_o^2 \; ; \qquad \lambda_1^2 = \frac{9}{4}$$

$$\tau_2^2 = -(k_2a_o)^2 = \frac{8}{9} - z_o^2 \; ; \qquad \lambda_2^2 = \frac{16}{9}$$

(53)

$$\tau_3^2 = -(k_3a_o)^2 = \frac{15}{16} - z_o^2; \qquad \lambda_3^2 = \frac{25}{16}$$

$$z_o = k_oa_o = .271\sqrt{\text{volts}}$$

and $0 < \text{volts} < 10$, so that $z_o^2 < .734$.

The evaluation of $N_1(\lambda,\tau)$ is carried out in appendix AV. From it the quantities $N_2 \ldots N_6$ and J are obtained through the relations (52). The results, in a form convenient for calculation, are

$$
(54)\quad \begin{cases}
N_1(\lambda,\tau) = \dfrac{1}{\lambda}\,\dfrac{1}{[z_o^2+(\tau+\lambda)^2]} \\[2ex]
N_2(\lambda,\tau) = -\dfrac{\partial N_1}{\partial \lambda^2} = \dfrac{N_1}{2\lambda^2} + (\tau+\lambda)N_1^2 \\[2ex]
N_3(\lambda,\tau) = -\dfrac{1}{2}\dfrac{\partial N_2}{\partial \lambda^2} = \dfrac{1}{4\lambda^2}\left[N_2 + \dfrac{N_1}{\lambda^2} - \lambda N_1^2 + 4N_1N_2\lambda^2(\tau+\lambda)\right] \\[2ex]
N_4(\lambda,\tau) = -\dfrac{1}{3}\dfrac{\partial N_3}{\partial \lambda^2} = \dfrac{1}{6\lambda^2}\Bigg[2N_3 + \dfrac{3}{4}\dfrac{N_2}{\lambda^2} + \dfrac{3}{4}\dfrac{N_1}{\lambda^4} - 2\lambda N_1N_2 \\[2ex]
\qquad\qquad + (\tau+\lambda)\left\{2\lambda^2N_2^2 + 4\lambda^2N_1N_3 - N_1N_2\right\}\Bigg] \\[2ex]
N_5(\lambda,\tau) = -\dfrac{1}{4}\dfrac{\partial N_4}{\partial \lambda^2} = \dfrac{1}{8\lambda^2}\Bigg[4N_4 + \dfrac{N_2}{2\lambda^4} + \dfrac{N_3}{2\lambda^2} + \dfrac{N_1}{2\lambda^6} + \dfrac{N_1N_2}{2\lambda} - 2\lambda N_1N_3 \\[2ex]
\qquad\qquad - \lambda N_2^2 + (\tau+\lambda)\left\{4\lambda^2N_2N_3 + 4\lambda^2N_1N_4 - 2N_1N_3 - N_2^2\right\}\Bigg] \\[2ex]
N_6(\lambda,\tau) = -\dfrac{1}{5}\dfrac{\partial N_5}{\partial \lambda^2} = \dfrac{1}{10\lambda^2}\Bigg[6N_5 + \dfrac{3N_1}{8\lambda^8} + \dfrac{3N_2}{8\lambda^6} + \dfrac{3N_3}{8\lambda^4} + \dfrac{3N_4}{8\lambda^2} \\[2ex]
\qquad\qquad + \dfrac{N_1N_2}{16\lambda^3} + \dfrac{3N_1N_3}{4\lambda} + \dfrac{3N_2^2}{8\lambda} - 2\lambda N_1N_4 - \dfrac{3\lambda N_2N_3}{2} \\[2ex]
\qquad\qquad + (\tau+\lambda)\left\{4\lambda^2N_2N_4 + 4\lambda^2N_1N_5 + 2\lambda^2N_3^2 - \dfrac{5}{2}N_2N_3 - \dfrac{5}{2}N_1N_4\right\}\Bigg] \\[2ex]
J(\lambda,\tau) = \displaystyle\int_0^{\lambda^2} N_1(\lambda,\tau)\,d\lambda^2 = \dfrac{2}{z_o}\tan^{-1}\dfrac{\lambda z_o}{z_o^2+\tau(\lambda+\tau)} \quad .
\end{cases}
$$

The following table presents numerical results for I_1, I_2, and I_3 in the energy range 0 - 10 volts, based on (51) through (54):

Table 2 (units of $4\pi a_o$)

volts	z_o	I_1	I_2	I_3	I_4
.135	.1	.966	.167	.060	$\sim$.029
.54	.2	.970	.171	.061	$\sim$.029
1.21	.3	.984	.171	.061	$\sim$.029
3.38	.5	1.001	.177	.063	$\sim$.029
6.75	.707	1.090	.187	.068	$\sim$.029
9.45	.835	1.227	.204	.071	$\sim$.029

The values of the factors in front of the brackets in (51) are $\frac{2^{16}}{3^{10}} = 1.110$, $\frac{3^6}{2^{12}} = .178$, and $\frac{9 \cdot 10^{23}}{5^{13}} = .062$, so that it appears from Table 2 that the complicated brackets in (51) are of the order unity in the energy range considered. We have made use of this fact in estimating the contribution of I_4. We have shown that I_4 can be written as

$$I_4 = (4\pi a_o) \frac{2^4 \cdot 5^7}{3^{16}} [\ldots.] \tag{55}$$

where the brackets in (55) contain terms much the same in form as those in the brackets of I_1, I_2, and I_3. Assuming the brackets here, too, contribute an amount of the order unity, then $I_4 \sim \frac{2^4 \cdot 5^7}{3^{16}} = .029$ (units of $4\pi a_o$).

Table 2 indicates the rapid convergence of the contributions from the higher discrete states. In fact (49) and (50) show that these contributions should fall off as $\frac{1}{n^3}$ for large principal quantum number n. We have, therefore, proceeded no farther than the fourth excited state.

It is interesting to observe that aside from a factor of 2, the factors $\frac{2^{16}}{3^{10}}$, $\frac{3^6}{2^{12}}$, $\frac{9 \cdot 2^{23}}{5^{13}}$, and $\frac{2^4 \cdot 5^7}{3^{16}}$ contained in I_1, I_2, I_3, and I_4, respectively, are generated by the formula

$$\frac{2^8}{3} \frac{(n+1)^7 \, n^{2n-3}}{(n+2)^{2n+7}} \qquad (n = 1,2,\ldots) \quad . \tag{56}$$

This expression is precisely the intensity formula for the spectral lines in the Lyman series of the hydrogen atom[31]. It thus appears that the contributions of the excited states to the denominator of (9), for $\theta = 0$, are in the same ratio, approximately, as the ratio of the Lyman series line intensities. This is not surprising, since inelastic collision probabilities (in this case virtual transitions from ground state to higher states) are intimately related to optical transition probabilities between the states[32].

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31. Bethe, loc.cit., p. 345.
32. Elsasser, Z.f. Phys. 45, 522 (1927).

B. Contribution of the Continuum States

The contribution of the continuum is determined by the quantity (see (37))

$$I_c = \frac{2a^2}{\pi}\int_0^\infty dk \int \frac{d\tau_{k'}}{(k'^2-k_c^2)K^4}\,|\varepsilon_{o,k}(K)|^2 \tag{57}$$

where

$$k_c^2 = k_o^2 - \frac{1}{a_o^2}\,[1+(ka_o)^2]$$

$$K^2 = k_o^2 + k'^2 - 2k'k_o \cos\lambda$$

$$d\tau_{k'} = k'^2 dk' \sin\lambda\, d\lambda\, d\beta$$

$$\vec{K} = k_o\vec{n}_o - \vec{k}'$$

and $|\varepsilon_{o,k}(K)|^2$ is given in (49).

We shall change integration variable from $\vec{k}'$ to $-\vec{K} = \vec{k}' - k_o\vec{n}_o$ in accordance with figure 3.

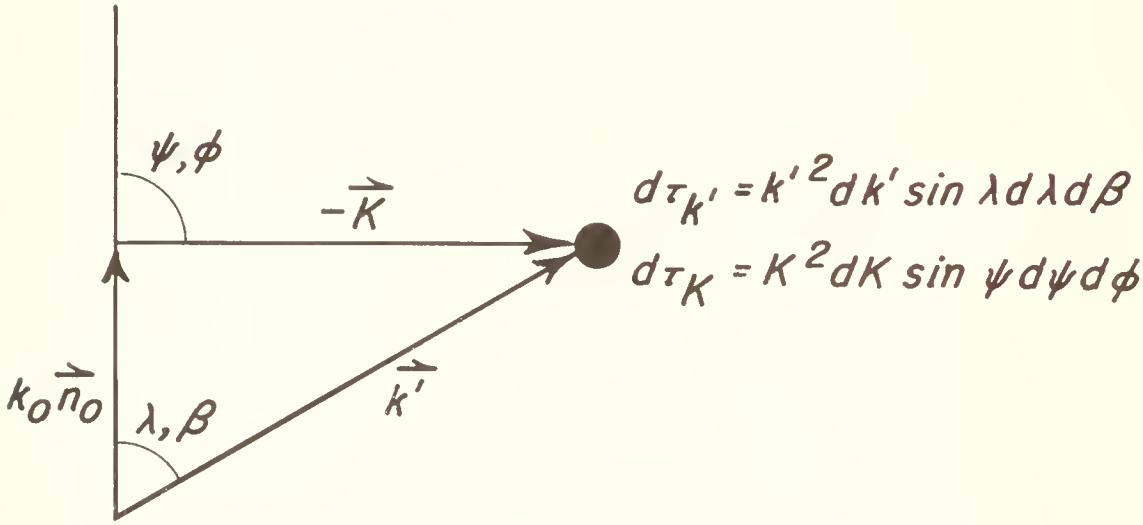

Fig. 3

Clearly

$$d\tau_{k'} = d\tau_K$$

and

$$k'^2 = k_o^2 + K^2 + 2Kk_o \cos\psi \quad .$$

Then we may write (57) as

$$I_c = \frac{2a^2}{\pi} \cdot \frac{2\pi}{2k_o} \int_0^\infty dk \int_0^\infty \frac{dK}{K^3} |\varepsilon_{o,k}(K)|^2 \int_{-1}^{1} \frac{dw}{\frac{K^2+k_o^2-k_c^2}{2Kk_o} + w} \quad (w = \cos\psi).$$

Noting that $\frac{K^2+k_o^2-k_c^2}{2Kk_o} > 1$ since $k_c^2 < 0$ in the energy range being considered, we obtain

$$I_c = \frac{2a^2}{k_o} \int_0^\infty dk \int_0^\infty \frac{dK}{K^3} |\varepsilon_{o,k}(K)|^2 \ln \frac{(K+k_o)^2-k_c^2}{(K-k_o)^2-k_c^2} \quad .$$

If now we use (49) in the last expression and introduce dimensionless quantities, we may write for the continuum contribution

$$(58) \qquad I_c = (4\pi a_o)\left(\frac{1}{\pi z_o}\right) \int_0^\infty z\,dz \int_0^\infty F(z,Z,z_o)\,dZ$$

where

$$(59) \quad F(z,Z,z_o) = \frac{512[Z^2 + \frac{1}{3}(1+z^2)]}{Z[(Z+z)^2+1]^3[(Z-z)^2+1]^3}$$

$$\cdot \frac{e^{-\frac{2}{z}\tan^{-1}\frac{2z}{Z^2-z^2+1}}}{1-e^{-2\pi/z}} \ln \frac{(Z+z_o)^2-z_c^2}{(Z-z_o)^2-z_c^2}$$

where

$$z_o = k_o a_o = .271\sqrt{\text{volts}}$$

$$z_c = k_c a_o$$

$$z = ka_o$$

$$Z = Ka_o$$

$$z_c^2 = z_o^2 - \left\{1 + z^2\right\} \quad .$$

(58) has been evaluated by numerical integration, for the six energies listed in table 2. For given z_o, different values of z were taken and $\int_0^\infty F(z,Z,z_o)dZ$ was graphically determined for each z. The quantity $z\int_0^\infty F(z,Z,z_o)dZ$ was then plotted as a function of z and the final area $\int_0^\infty z\int_0^\infty F(z,Z,z_o)dZdz$ determined.

The convergence of the integrand in (58) in both z and Z is extremely rapid and in no case was it necessary to go beyond z or Z = 5 in taking areas. In fact, the upper limit 3 in the z and Z integrations sufficed most of the time. From (59) we see that

$$(60) \qquad F \sim \frac{2048z_o}{1-e^{-2\pi/z}} \cdot \frac{1}{Z^{12}} \quad \text{for } z_o,\ z \text{ fixed and } Z \text{ large}$$

and

$$(61) \qquad zF \sim \frac{2048z_o}{2\pi} \cdot \frac{1}{z^{10}} \quad \text{for } z_o,\ Z \text{ fixed and } z \text{ large} \quad .$$

Thus, for example, at 3.38 volts (z_o = .5) and with z = 1, (60) gives

$$\int_5^\infty F(z,Z,z_o)dZ = \frac{1024}{1-e^{-2\pi}} \frac{1}{11 \cdot 5^{11}} \sim \frac{1}{5^8}$$

giving an error only in the sixth significant figure in the overall area from 0 to ∞. On the other hand, at $Z = 3$ the <u>correct</u> value of F is .0013, while (60) gives $\sim$ .002, so that certainly the error incurred in integrating from $Z = 0$ to $Z = 3$ will be <u>less</u> than $\int_3^\infty FdZ$ with F given by (60):

$$\int_3^\infty F(z,Z,z_o)dZ = \frac{1024}{1-e^{-2\pi}} \frac{1}{11 \cdot 3^{11}} \sim .0006 \quad ,$$

or an error in the fourth significant figure.

Table 3 presents the numerical results of the contributions from the higher discrete states, the continuum, and the ground state term I_o (see eq. (43)). The continuum contribution is quoted to three place accuracy. The last column in Table 3 presents the final value for $I(0) = I_o + \sum_{n>0} I_n + I_c$ (see (37)):

Table 3 (units of $4\pi d_o$)

volts	z_o	I_o	I_1	I_2	I_3	I_4	I_c	$I(0)$
.135	.1	.769+i(.099)	.966	.167	.060	~.029	.783	2.774+i(.099)
.54	.2	.734+i(.189)	.970	.171	.061	~.029	.788	2.753+i(.189)
1.21	.3	.683+i(.264)	.984	.171	.061	~.029	.793	2.720+i(.264)
3.38	.5	.554+i(.361)	1.001	.177	.063	~.029	.815	2.639+i(.361)
6.75	.707	.425+i(.397)	1.090	.187	.068	~.029	.837	2.636+i(.397)
9.45	.835	.357+i(.397)	1.227	.204	.071	~.029	.879	2.767+i(.397)

Based on Table 3, the total elastic cross-section for the complete scattering can be obtained. From eqs. (9) and (44)

$$f_o(0) = \frac{a_o}{1 + \frac{I(0)}{-4\pi a_o}}$$

with

$$Q = \frac{4\pi}{k_o} \operatorname{Im} f_o(0) \quad .$$

Table 4 gives the final results:

Table 4 (cross-sections in units of $4\pi a_o^2$)

volts	z_o	Q complete
.135	.1	.31
.54	.2	.30
1.21	.3	.29
3.38	.5	.26
6.75	.707	.20
9.45	.835	.15

VI. Discussion of Results and Conclusions

The results presented in table 4 shows cross-sections a good deal smaller than those for scattering from the static field (Table 1). This follows the trend exhibited by the work of other authors[33]. However, our cross-sections are even smaller than those given by Massey and Moiseiwitsch[33].

This is somewhat surprising in that better results for the complete scattering were anticipated on the basis of the success of the method for the static field scattering. This inconsistency is attributable to the use of Born trial fields in the low energy range 0 - 10 volts. Such an approximation is equivalent to the use of a Born trial field for each of the virtual inelastic waves from the higher atomic states, and the accumulation of errors is apparently large.

It is quite conceivable that at higher energies Born trial fields would give far better results. We have not considered energies outside the 0 - 10 volt range for several reasons: collisions between electrons and atomic systems in the upper atmosphere occur at very low incident energies; and for incident energies greater than 10.17 volts physical excitation of the higher atomic states is possible, in which case the mathematical complexities of the calculation increase, for then the singularities in the integrands of I_n and I_c (eqs. (50) and (57)) are distributed along the real axis as well

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33. See, for example, Massey and Moiseiwitsch, Proc. Roy. Soc. A205, 483 (1951); table 3, column on the exchange-polarization approximation.

as the imaginary axis in the k' plane and the numerical evaluation of I_c would then be especially complicated. In this case, the cross-section Q given by equation (11) represents the sum of the total elastic and all the total inelastic cross-sections.

The results are of definite interest in that they indicate the vital roles played by the excited states and the continuum in the elastic scattering (table 3). For example, at 6.75 volts table 3 indicates that the first four discrete states contribute 52% and the continuum 32% to the denominator of the Schwinger variational expression (eq. (9)), the balance arising from the ground state.

Physically, the virtual transitions of the atom to the higher states during the collision can be thought of as arising from the interaction presented by the incident electron. Thus, though the incident electron has insufficient energy for physical excitation of the atom, in a quantum mechanical sense the atom can not be regarded as strictly in the 1S state during the collision. One can say that the incident electron distorts the 1S charge distribution into a form which must be accounted for by the possibility of the electron being in all higher atomic states, including the continuum, even though physical measurement could not detect it there. In this sense, these virtual transitions are related to the polarization of the charge distribution by the incident electron.

We feel, therefore, that in any description of the elastic scattering it is completely inadequate to assume merely static field scattering since the higher states contribute so importantly to the polarization field. We feel, also, that in a more exact theory of calculating cross-sections, the evaluation of their contributions may well have to proceed along the lines indicated in this paper.

Of definite interest also is the tractability of the difficult integrals involving Green's functions inherent in the Schwinger variational method.

The use of a Born trial field represents one extreme in an approximation scheme. At the other extreme would be the use[34] of H^- wave functions in which the incident electron as well as the atomic electron are regarded as bound to the proton. The wave function is then of the form $e^{-\alpha r_1} e^{-\beta r_2}$ times a polynomial in r_1 and r_2. The evaluation of the stationay expression (4) is then far more complex. Inasmuch as the incident electron spends considerable time in the vicinity of the atom, we would expect the general conclusions regarding the contributions of the excited states and the continuum to carry over, in spite of the rapid vanishing of this wave function as r_1 and r_2 increase over the domain of the atom.

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34. This was brought to our attention by Dr. S. Altshuler, (private communication).

Appendix A-I

Evaluation of $\int e^{i\vec{K}\cdot\vec{r}} |\phi_o(\vec{r})|^2 d\tau$:

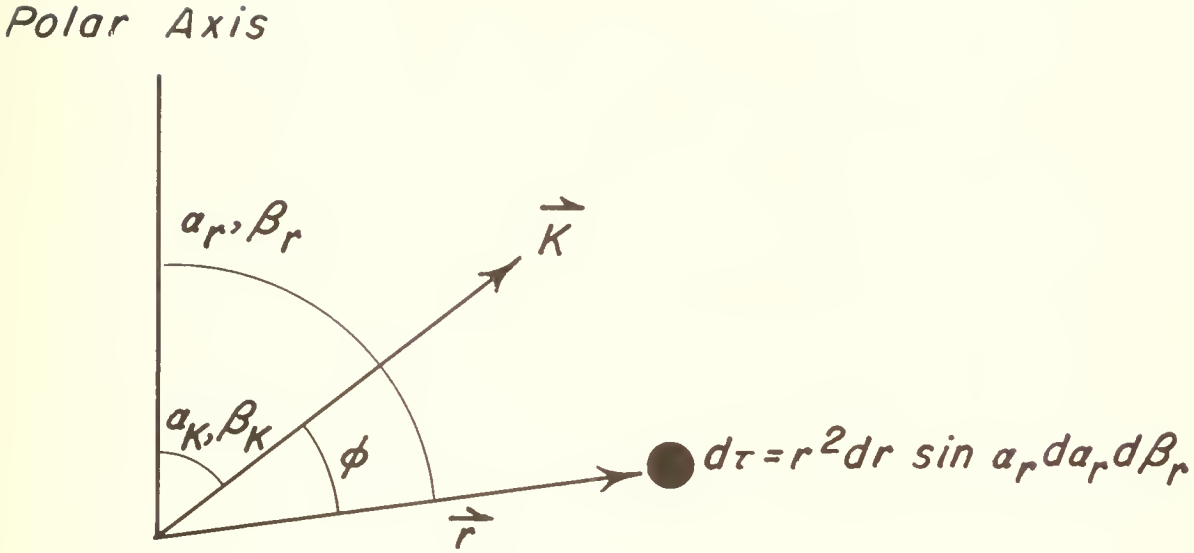


Fig. 4

Using the expansion[35]

$$e^{i\vec{K}\cdot\vec{r}} = \sum_{\ell=0}^{\infty} (2\ell+1) i^{\ell} j_{\ell}(Kr) P_{\ell}(\cos\phi) \quad ,$$

where $j_{\ell}(Kr)$ are the spherical Bessel functions and $P_{\ell}(\cos\phi)$ the Legendre polynomials, we have (see fig. 4)

$$\text{(AI-1)} \quad \int e^{i\vec{K}\cdot\vec{r}} |\phi_o(\vec{r})|^2 d\tau = \sum_{\ell=0}^{\infty} (2\ell+1) i^{\ell} j_{\ell}(Kr) P_{\ell}(\cos\phi) \, |\phi_o(\vec{r})|^2 r^2 dr \sin\alpha_r \, d\alpha_r \, d\beta_r$$

35. L. I. Schiff, loc.cit. p. 105, p. 173.

If we use the identity[35]

$$\text{(AI-2)} \quad P_\ell(\cos\phi) = P_\ell(\cos\alpha_K)P_\ell(\cos\alpha_r)$$

$$+ 2\sum_{\mu=1}^{\ell} \frac{(\ell-\mu)!}{(\ell+\mu)!} P_\ell^\mu(\cos\alpha_K)P_\ell^\mu(\cos\alpha_r)\cos\mu(\beta_r-\beta_K)$$

where P_ℓ^μ are the associated Legendre polynomials, and the orthogonality of the Legendre polynomials

$$\int_{-1}^{1} P_\ell(w)P_{\ell'}(w)dw = \frac{2}{2\ell+1}\delta_{\ell\ell'} \quad , \quad (w = \cos\alpha_r) \quad ,$$

and

$$\int_0^{2\pi} \cos\mu(\beta_r-\beta_K)d\beta_r = 0 \quad (\mu > 0) \quad ,$$

and $P_o(w) = 1$, then (AI-1) becomes

$$\int e^{i\vec{K}\cdot\vec{r}} |\phi_o(\vec{r})|^2 d\tau = 4\pi\int_0^\infty j_o(Kr)|\phi_o(\vec{r})|^2 r^2 dr \quad .$$

With

$$j_o(Kr) = \frac{\sin Kr}{Kr} \quad \text{and} \quad \phi_o(\vec{r}) = \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o}$$

we have

$$\int e^{i\vec{K}\cdot\vec{r}} |\phi_o(\vec{r})|^2 d\tau = \frac{a^3}{2K}\int_0^\infty r e^{-\alpha r} \sin Kr dr$$

$$= \frac{a^4}{(K^2+a^2)^2} \quad ; \quad \alpha = 2/a_o \quad .$$

Appendix A-II

Evaluation of Static Field $W_{oo}(\vec{r}_1)$:

$$W_{oo}(\vec{r}_1) = \frac{2}{a_o}\int\left(\frac{1}{r_{12}} - \frac{1}{r_1}\right)|\phi_o(\vec{r}_2)|^2 d\tau_2$$

where

$$\phi_o(\vec{r}_2) = \frac{1}{\sqrt{\pi a_o^3}}\, e^{-r_2/a_o} = \text{ground state hydrogen wave function .}$$

The integration is performed in accordance with figure 5.

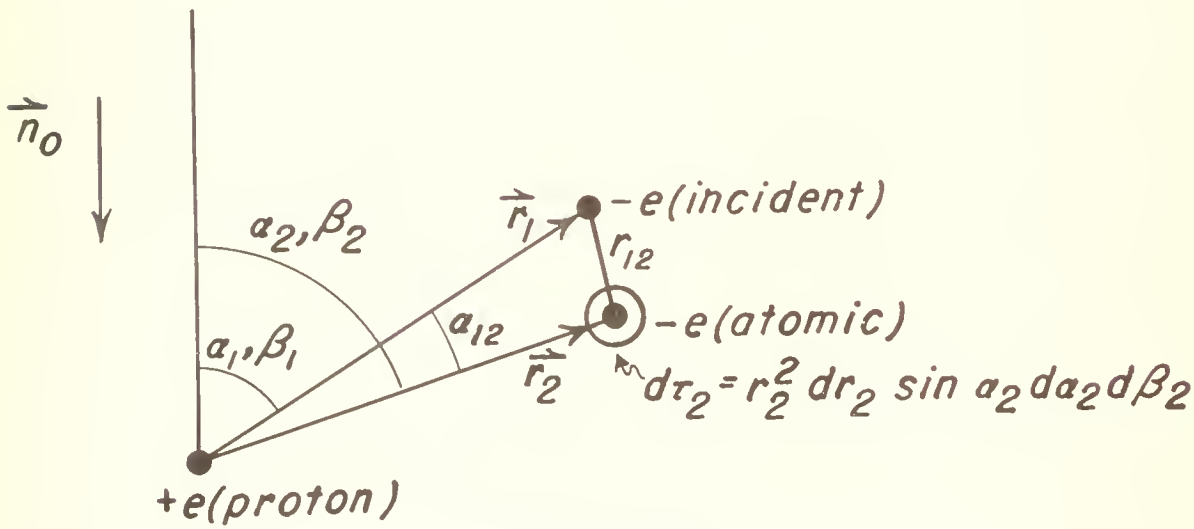


Fig. 5

Expanding $\frac{1}{r_{12}}$ in spherical harmonics[36] and using the normality of the hydrogen wave functions, we have

36. L. I. Schiff, loc.cit. p. 173.

$$W_{oo}(\vec{r}_1) = \frac{2}{a_o}\frac{1}{\pi a_o^3}\left[\int_0^{r_1}\int_0^{\pi}\int_0^{2\pi}\frac{1}{r_1}\sum_{\ell=0}^{\infty}\left(\frac{r_2}{r_1}\right)^{\ell} P_{\ell}(\cos\alpha_{12})e^{-2r_2/a_o}\right.$$

$$\cdot\, r_2^2\, dr_2 \sin\alpha_2\, d\alpha_2 d\beta_2$$

$$+\int_{r_1}^{\infty}\int_0^{\pi}\int_0^{2\pi}\frac{1}{r_2}\sum_{\ell=0}^{\infty}\left(\frac{r_1}{r_2}\right)^{\ell} P_{\ell}(\cos\alpha_{12})e^{-2r_2/a_o}$$

$$\left.\cdot\, r_2^2\, dr_2 \sin\alpha_2\, d\alpha_2 d\beta_2\right] - \frac{2}{a_o r_1} \quad .$$

If now we use the expansion (AI-2) (where $\phi \rightarrow \alpha_{12}$, $\alpha_K \rightarrow \alpha_1$, $\beta_K \rightarrow \beta_1$, $\alpha_r \rightarrow \alpha_2$, $\beta_r \rightarrow \beta_2$) and the same arguments as those following (AI-2), we obtain

$$W_{oo}(\vec{r}_1) = \frac{8}{a_o^4}\left[\int_0^{r_1}\frac{r_2^2}{r_1}e^{-2r_2/a_o}\,dr_2 + \int_{r_1}^{\infty} r_2\, e^{-2r_2/a_o}\,dr_2\right] - \frac{2}{a_o r_1} \quad .$$

The remainder of the integrations are elementary and the result for the static field potential is

$$W_{oo}(r) = -\frac{2}{a_o}\left(\frac{1}{a_o} + \frac{1}{r}\right) e^{-2r/a_o} \quad .$$

Appendix A-III

Evaluation of $-\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(r)d\tau$:

The integration is performed with the polar axis along $\vec{K}$ as in figure 6.

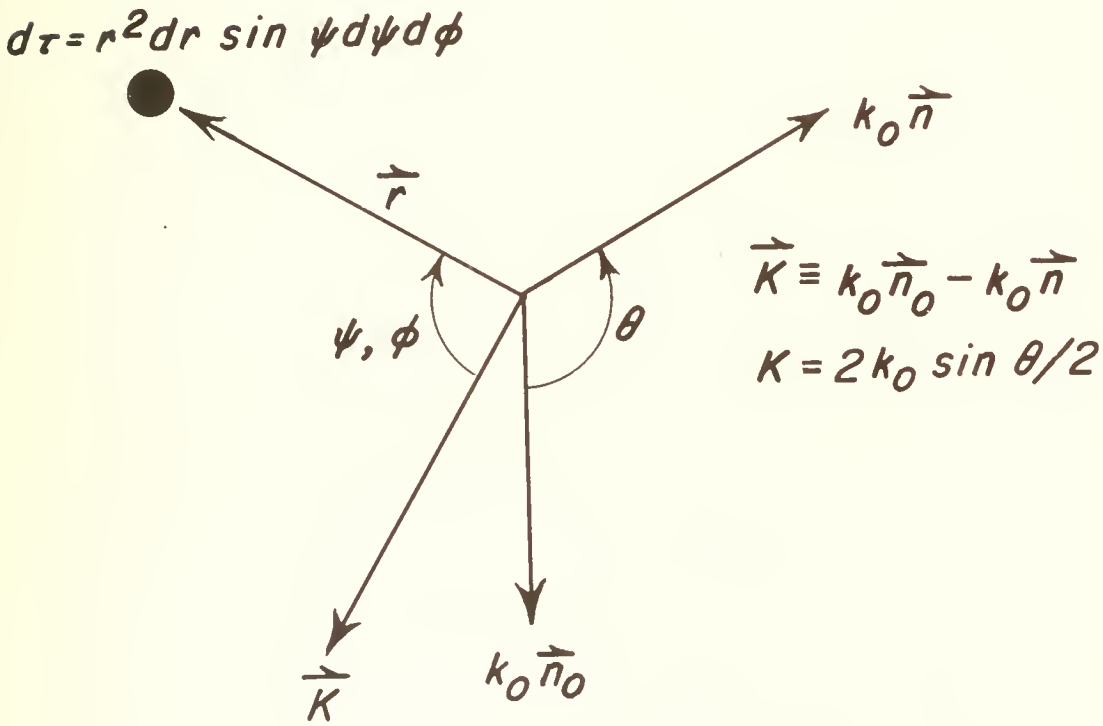


Fig. 6

Then

$$-\frac{1}{4\pi}\int e^{ik_o(\vec{n}_o-\vec{n})\cdot\vec{r}}\, W_{oo}(r)d\tau = -\frac{1}{4\pi}\int e^{i\vec{K}\cdot\vec{r}}\, W_{oo}(r)r^2dr \sin\psi\, d\psi d\phi$$

$$= -\frac{1}{2}\int_0^\infty W_{oo}(r)r^2dr\int_{-1}^{1} e^{iKrw}\, dw \quad (w = \cos\psi)$$

$$= -\int_0^\infty W_{oo}(r)\ \frac{\sin Kr}{Kr} \cdot r^2 dr$$

$$= \frac{2}{a_o}\int_0^\infty \left(\frac{1}{a_o} + \frac{1}{r}\right) e^{-2r/a_o} \cdot \frac{\sin Kr}{K} \cdot r\, dr$$

$$= \alpha\ \frac{(2\alpha^2 + K^2)}{(\alpha^2 + K^2)^2} \quad ; \quad \alpha = \frac{2}{a_o} \quad ; \quad K = 2k_o \sin\frac{\theta}{2} \quad .$$

Appendix A-IV

Evaluation of $D(0) = I_o = \frac{2\alpha^2}{\pi}\int \frac{d\tau_{k'}}{k'^2-k_o^2}\,\frac{(2\alpha^2+K^2)^2}{(\alpha^2+K^2)^4}$:

$$K^2 = k'^2 + k_o^2 - 2k'k_o\cos\lambda \quad \text{and} \quad d\tau_{k'} = k'^2 dk' \sin\lambda\, d\lambda d\beta \quad .$$

Setting

$$w = \cos\lambda\ , \quad A = \alpha^2 + k'^2 + k_o^2\ , \quad B = 2k'k_o\ ,$$

$$A + B = \alpha^2 + (k'+k_o)^2\ , \quad A - B = \alpha^2 + (k'-k_o)^2\ ,$$

we may write

$$D(0) = \frac{2\alpha^2}{\pi}\int \frac{k'^2 dk' dw d\beta}{(k'^2-k_o^2)}\,\frac{(\alpha^2+A-Bw)^2}{(A-Bw)^4}$$

$$= 4\alpha^2\int_0^\infty \frac{k'^2 dk'}{(k'^2-k_o^2)}\left[\int_{-1}^{1}\frac{\alpha^4 dw}{(A-Bw)^4} + \int_{-1}^{1}\frac{2\alpha^2 dw}{(A-Bw)^3} + \int_{-1}^{1}\frac{dw}{(A-Bw)^2}\right]$$

Carrying through the w integrations we obtain

$$D(0) = \frac{2\alpha^2}{k_o}\int_0^\infty \frac{k'dk'}{(k'^2-k_o^2)}\left[\frac{\alpha^4}{3[\alpha^2+(k'-k_o)^2]^3} - \frac{\alpha^4}{3[\alpha^2+(k'+k_o)^2]^3}\right]$$

$$+ \frac{2\alpha^2}{k_o}\int_0^\infty \frac{k'dk'}{(k'-k_o^2)}\left[\frac{\alpha^2}{[\alpha^2+(k'-k_o)^2]^2} - \frac{\alpha^2}{[\alpha^2+(k'+k_o)^2]^2}\right]$$

$$+ \frac{2\alpha^2}{k_o}\int_0^\infty \frac{k'dk'}{(k'^2-k_o^2)}\left[\frac{1}{[\alpha^2+(k'-k_o)^2]} - \frac{1}{[\alpha^2+(k'+k_o)^2]}\right] \quad .$$

By making the substitution $k' = -z$ in the second integrals in each of the above terms we find

$$D(0) = \frac{2}{3}\frac{a^6}{k_o}\int_{-\infty}^{\infty} \frac{k'dk'}{(k'^2-k_o^2)} \cdot \frac{1}{[a^2+(k'-k_o)^2]^3}$$

$$+ \frac{2a^4}{k_o}\int_{-\infty}^{\infty} \frac{k'dk'}{(k'^2-k_o^2)} \cdot \frac{1}{[a^2+(k'-k_o)^2]^2}$$

$$+ \frac{2a^2}{k_o}\int_{-\infty}^{\infty} \frac{k'dk'}{(k'^2-k_o^2)} \cdot \frac{1}{[a^2+(k'-k_o)^2]}$$

which we shall write as

$$\text{(AIV-1)} \quad D(0) = \frac{a^6}{3} N_3 + a^4 N_2 + a^2 N_1$$

where

$$\text{(AIV-2)} \qquad N_i = \frac{2}{k_o}\int_{-\infty}^{\infty} \frac{k'dk'}{(k'^2-k_o^2)} \cdot \frac{1}{[a^2+(k'-k_o)^2]^i}, \quad (i = 1,2,3)$$

and

$$\text{(AIV-3)} \qquad N_3 = -\frac{1}{4a}\frac{\partial N_2}{\partial a}, \quad N_2 = -\frac{1}{2a}\frac{\partial N_1}{\partial a} .$$

We, therefore, have only to calculate the integral

$$N_1 = \frac{2}{k_o}\int_{-\infty}^{\infty} \frac{k'dk'}{(k'^2-k_o^2)} \cdot \frac{1}{[a^2+(k'-k_o)^2]} .$$

This we shall do in the complex k' plane, recalling the remarks made after equation (18), section III, concerning the contour (see fig. 1).

The singularities in the integrand of N_1 occur at $k' = \pm k_o$, $k' = k_o \pm i\alpha$ (see fig. 7).

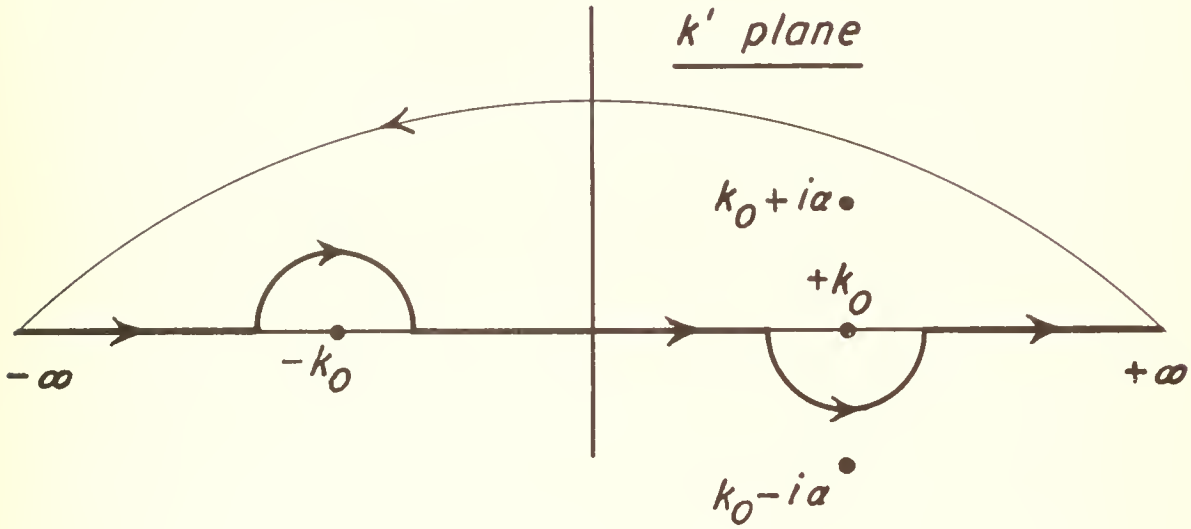


Fig. 7

On the infinite arc, the integrand of N_1 vanishes so that we may write

$$N_1 = \frac{2}{k_o} \oint \frac{\dfrac{k'dk'}{(k'+k_o)(k'-k_o+i\alpha)}}{(k'-k_o)(k'-k_o-i\alpha)}$$

$$= \frac{2i}{k_o\alpha}\left[\oint \frac{\dfrac{k'dk'}{(k'+k_o)(k'-k_o+i\alpha)}}{(k'-k_o)} - \oint \frac{\dfrac{k'dk'}{(k'+k_o)(k'-k_o+i\alpha)}}{[k'-(k_o+i\alpha)]}\right] .$$

Applying Cauchy's integral theorem

$$\oint \frac{f(k')dk'}{k'-a} = 2\pi i\ f(a) \quad \text{(a within the contour)}$$

to each of the above integrals, we find after some algebra

(AIV-4) $$N_1 = \frac{2\pi}{\alpha(4k_o^2+\alpha^2)} + i\,\frac{4\pi k_o}{\alpha^2(4k_o^2+\alpha^2)}$$

We could equally well have chosen the infinite arc in the lower half plane. The result, of course, is the same.

From (AIV-3) and (AIV-4) we find

(AIV-5)
$$N_2 = \frac{\pi}{\alpha^3}\left[\frac{4k_o^2+3\alpha^2}{(4k_o^2+\alpha^2)^2} + i4k_o\,\frac{4k_o^2+2\alpha^2}{\alpha(4k_o^2+\alpha^2)^2}\right]$$

$$N_3 = \frac{\pi}{4\alpha^5}\left[\frac{48k_o^4+40\alpha^2k_o^2+15\alpha^4}{(4k_o^2+\alpha^2)^3} + i16k_o\,\frac{16k_o^4+12k_o^2\alpha^2+3\alpha^4}{\alpha(4k_o^2+\alpha^2)^3}\right]$$

With (AIV-4) and (AIV-5), (AIV-1) gives for D(0):

$$D(0) = I_o = 4\pi a_o\left[\frac{39(k_oa_o)^4+106(k_oa_o)^2+75}{96[1+(k_oa_o)^2]^3}\right.$$

$$\left. + i\,\frac{k_oa_o}{12}\cdot\frac{7(k_oa_o)^4+18(k_oa_o)^2+12}{[1+(k_oa_o)^2]^3}\right]$$

Appendix A-V

Evaluation of $I_2 = \frac{2a^2}{\pi}\int \frac{d\tau_{k'}}{(k'^2-k_2^2)K^4}\,|\varepsilon_{o,2}(K)|^2$:

From equation (49)

$$|\varepsilon_{o,2}(K)|^2 = \frac{K^2 a^8 3^{-3}(\frac{2}{27}\,a^2+K^2)}{(\frac{4}{9}\,a^2+K^2)^6} \quad .$$

So

$$\text{(AV-1)} \quad I_2 = \frac{4a^{12}}{3^6\cdot\pi}\int \frac{d\tau_{k'}}{(k'^2+\sigma_2^2)}\left[\frac{1}{K^2(\gamma_2^2+K^2)^6} + \frac{6}{\gamma_2^2}\,\frac{1}{(\gamma_2^2+K^2)^6}\right]$$

where $K^2 = k'^2 + k_o^2 - 2k'k_o \cos\lambda$ and

$$\text{(AV-2)} \quad \begin{aligned} \sigma_2^2 &\equiv -k_2^2 = \frac{8}{9a_o^2} - k_o^2 > 0 \quad \text{for energies less than 10 volts} \\ \gamma_2^2 &\equiv \frac{4}{9}\,a^2 = \frac{16}{9a_o^2} \quad . \end{aligned}$$

Setting

$$A = k'^2 + k_o^2, \quad B = 2k'k_o, \quad A' = \gamma_2^2 + k'^2 + k_o^2 \ ,$$

$$A + B = (k' + k_o)^2, \quad A - B = (k' - k_o)^2 \ ,$$

$$A' + B = \gamma_2^2 + (k' + k_o)^2, \quad A' - B = \gamma_2^2 + (k' - k_o)^2 \ ,$$

$$A' - A = \gamma_2^2, \quad K^2 = A - Bw, \quad w = \cos\lambda \ ,$$

$$d\tau_{k'} = -k'^2 dk'\, dw\, d\beta$$

and expanding $\frac{1}{(A - Bw)(A' - Bw)^6}$ in partial fractions, (AV-1) becomes

$$I_2 = \frac{2^3 \cdot a^{12}}{3^6 \cdot \gamma_2^{12}} \int_0^{\infty} \int_{-1}^{1} \frac{k'^2 dk' dw}{(k'^2 + \sigma_2^2)} \left[\left(\frac{1}{A - Bw} - \frac{1}{A' - Bw} \right) - \frac{\gamma_2^2}{(A' - Bw)^2} \right.$$

$$\left. - \frac{\gamma_2^4}{(A' - Bw)^3} - \frac{\gamma_2^6}{(A' - Bw)^4} - \frac{\gamma_2^8}{(A' - Bw)^5} + \frac{5\gamma_2^{10}}{(A' - Bw)^6} \right] .$$

The w integrations are easily carried out and the result is

$$\text{(AV-3)} \quad I_2 = (4\pi a_o) \frac{a^{12}}{3^6 \cdot \gamma_2^{12}} \left[J - \gamma_2^2 N_1 - \frac{\gamma_2^4}{2} N_2 - \frac{\gamma_2^6}{3} N_3 - \frac{\gamma_2^8}{4} N_4 + \gamma_2^{10} N_5 \right]$$

where

$$\text{(AV-3a)} \quad N_i = \frac{1}{\pi k_o a_o} \int_{-\infty}^{\infty} \frac{k' dk'}{(k'^2 + \sigma_2^2)} \frac{1}{[\gamma_2^2 + (k' - k_o)^2]^i} \qquad (i = 1, \ldots, 5)$$

$$J = \frac{1}{\pi k_o a_o} \int_{-\infty}^{\infty} \frac{k' dk'}{(k'^2 + \sigma_2^2)} \ln \frac{\gamma_2^2 + (k' - k_o)^2}{(k' - k_o)^2} .$$

If we finally set

$$\text{(AV-4)} \quad z_o = k_o a_o, \quad \lambda_2^2 = (\gamma_2 a_o)^2 = \frac{16}{9}, \quad \tau_2^2 = (\sigma_2 a_o)^2 = \frac{8}{9} - z_o^2$$

and use the new variable of integration $\zeta = k' a_o$, then we may write (AV-3) as

$$\text{(AV-5)} \quad I_2 = (4\pi a_o) \frac{3^6}{2^{12}} \left[J - \lambda_2^2 N_1 - \frac{\lambda_2^4}{2} N_2 - \frac{\lambda_2^6}{3} N_3 - \frac{\lambda_2^8}{4} N_4 + \lambda_2^{10} N_5 \right]$$

where now

(AV-5a) $$N_i(\lambda_2,\tau_2) = \frac{1}{\pi z_o}\int_{-\infty}^{\infty} \frac{\zeta d\zeta}{(\zeta^2+\tau_2^2)} \frac{1}{[\lambda_2^2+(\zeta-z_o)^2]^i} \qquad (i=1,\ldots,5)$$

$$J(\lambda_2,\tau_2) = \frac{1}{\pi z_o}\int_{-\infty}^{\infty} \frac{\zeta d\zeta}{(\zeta^2+\tau_2^2)} \ln \frac{\lambda_2^2+(\zeta-z_o)^2}{(\zeta-z_o)^2}$$

We note that

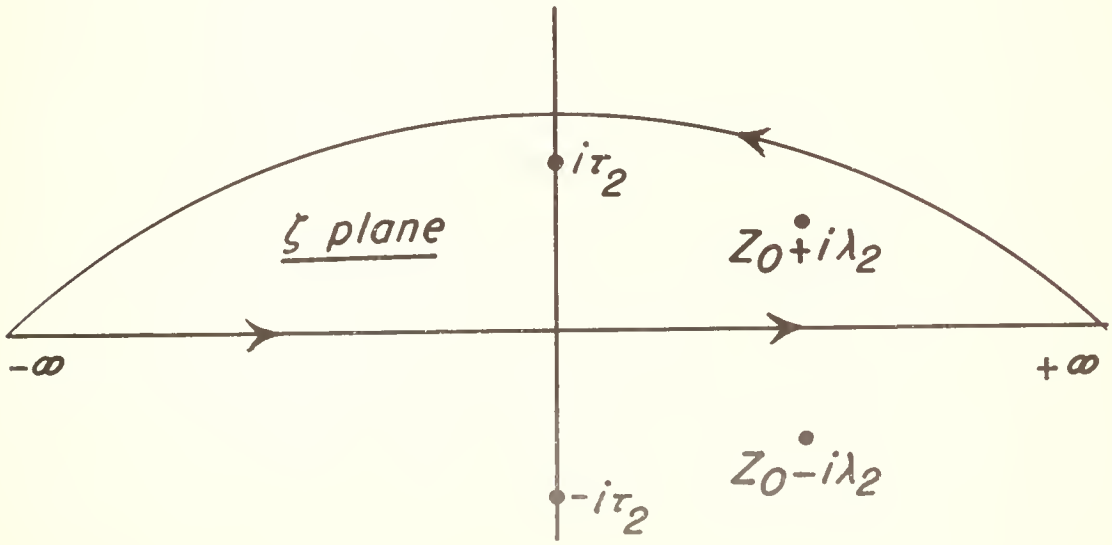
(AV-6) $$N_i = -\frac{1}{(i-1)}\frac{\partial N_{i-1}}{\partial \lambda_2^2} \quad (i = 2,\ldots,5)$$

$$J = \int_0^{\lambda_2^2} N_1(\lambda_2,\tau_2)d\lambda_2^2$$

We have, therefore, only to evaluate

(AV-7) $$N_1 = \frac{1}{\pi z_o}\int_{-\infty}^{\infty} \frac{\zeta d\zeta}{(\zeta^2+\tau_2^2)} \frac{1}{[\lambda_2^2+(\zeta-z_o)^2]}$$

This may be accomplished most conveniently in the complex ζ plane (fig. 8) in accordance with figure 1 and the remarks after equation (18) concerning imaginary values of k_m (i.e. $\tau_2^2 > 0$).



As the integrand of N_1 vanishes on the infinite arc, we may write

$$N_1 = \frac{1}{\pi z_o} \oint \frac{\dfrac{\zeta d\zeta}{(\zeta+i\tau_2)(\zeta-z_o+i\lambda_2)}}{(\zeta-i\tau_2)(\zeta-z_o-i\lambda_2)}$$

$$= \frac{1}{\pi z_o} \frac{1}{[i(\tau_2-\lambda_2)-z_o]} \left[\oint \frac{\dfrac{\zeta d\zeta}{(\zeta+i\tau_2)(\zeta-z_o+i\lambda_2)}}{(\zeta-i\tau_2)} - \oint \frac{\dfrac{\zeta d\zeta}{(\zeta+i\tau_2)(\zeta-z_o+i\lambda_2)}}{[\zeta-(z_o+i\lambda_2)]} \right] .$$

Using Cauchy's integral theorem in each of the two contour integrals, we find

$$\text{(AV-8)} \qquad N_1 = \frac{1}{\lambda_2[z_o^2+(\tau_2+\lambda_2)^2]} .$$

Then N_2 through N_5 and J are determined from (AV-6) and (AV-8):

$$N_2 = -\frac{\partial N_1}{\partial \lambda_2^2} = \frac{N_1}{2\lambda_2^2} + (\tau_2+\lambda_2)N_1^2$$

$$N_3 = -\frac{1}{2}\frac{\partial N_2}{\partial \lambda_2^2} = \frac{1}{4\lambda_2^2}\left[N_2 + \frac{N_1}{\lambda_2^2} - \lambda_2 N_1^2 + (\tau_2+\lambda_2)4\lambda_2^2 N_1 N_2\right]$$

$$N_4 = -\frac{1}{3}\frac{\partial N_3}{\partial \lambda_2^2} = \frac{1}{6\lambda_2^2}\left[2N_3 + \frac{3}{4}\frac{N_2}{\lambda_2^2} + \frac{3}{4}\frac{N_1}{\lambda_2^4} - 2\lambda_2 N_1 N_2 + (\tau_2+\lambda_2)\left\{2\lambda_2^2 N_2^2 + 4\lambda_2^2 N_1 N_3 - N_1 N_2\right\}\right]$$

$$N_5 = -\frac{1}{4}\frac{\partial N_4}{\partial \lambda_2^2} = \frac{1}{8\lambda_2^2}\Big[4N_4 + \frac{N_2}{2\lambda_2^4} + \frac{N_3}{2\lambda_2^2} + \frac{N_1}{2\lambda_2^6} + \frac{N_1N_2}{2\lambda_2} - 2\lambda_2 N_1 N_3 - \lambda_2 N_2^2$$

$$+ (\tau_2 + \lambda_2)\Big\{4\lambda_2^2 N_2 N_3 + 4\lambda_2^2 N_1 N_4 - 2N_1N_3 - N_2^2\Big\}\Big]$$

$$J = \int_0^{\lambda^2} N_1(\lambda_2, \tau_2)\, d\lambda_2^2 = \frac{2}{z_o}\tan^{-1}\frac{\lambda_2 z_o}{z_o^2 + \tau_2(\lambda_2 + \tau_2)}$$

with

$$\tau_2^2 = \frac{8}{9} - z_o^2\,, \quad \lambda_2^2 = \frac{16}{9}\,, \quad z_o = k_o a_o = .271\sqrt{\text{volts}}$$